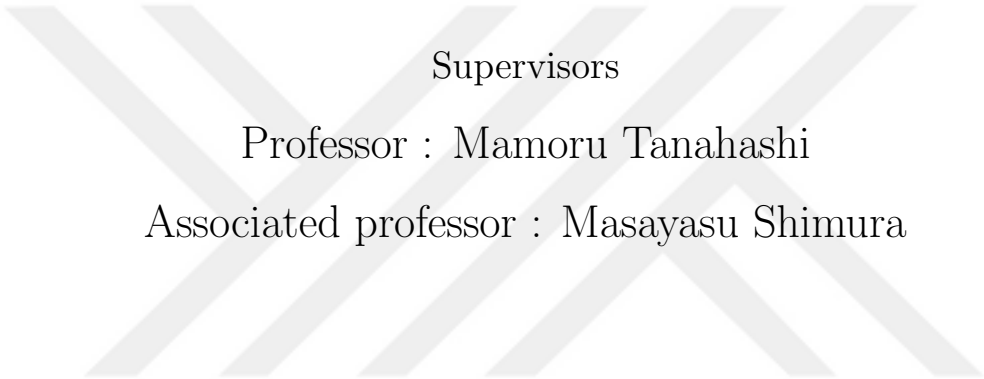


Doctoral Dissertation

Direct Numerical Simulations of Lifted Flames
of Hydrogen and Steam Diluted Oxygen



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Chapter 1

Introduction

1.1 Combustion in relation to current environmental issues

Even though there is an urging demand to replace fossil fuels with alternative energy sources, our lives still depend on the combustion of fossil fuels such as coal, oil, and natural gas. Figure 1.1 shows the primary energy consumption of the world by fuel [1]. Data up to the year 2019 are the energy consumption history of the world, and years after that show the future projections. By today, about 80% of the primary energy consumption is supplied by fossil fuels. Even though the percent usage of fossil fuels is predicted to decrease until 2050 (becoming around 68% of the total energy consumption), the total amount of fossil fuel consumption will increase as the total energy demand of the world increases.

As can be seen from Fig. 1.2, in the year 2019, power generation accounts for almost 40% of the total global energy consumption, and the percentage, as well as the total consumption amount, further increases in the following three decades [1]. Figure 1.3 shows the fuels used to supply the energy demand. Even though the projections show that the increased use of renewables can supply the increasing energy demand, fossil fuel consumption is also increased [1]. Therefore, it is necessary to develop environmentally

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friendly, safe, and efficient combustion technologies. For the last couple of decades, several technologies that can reach high efficiency while maintaining low emission levels have been developed. The exhaust gas recirculation (EGR) technique is designed to decrease NO_x emissions and thermal loss, and turbulent combustion is studied with high compression ratios, ultra-lean conditions, and high EGR ratios [2, 3]. EGR is also implemented in gas turbines [4]. Another technology used for practical combustion devices is the homogeneous charge compression ignition (HCCI) [5, 6].

Apart from developing new combustion technologies, using alternative fuels is another way to reduce the emissions of combustion devices. Hydrogen has been studied as an alternative fuel for decades since its combustion does not produce any CO_2 emissions. For the last 20 years, many practical gas turbines have been using H_2 as a fuel additive to decrease the CO_2 emissions [7, 8], but using pure H_2 as fuel is still being studied.

H_2 is two times more energy-dense than methane on a mass basis. However, it is three times less energy-dense than methane on a volume basis, which means that three times more H_2 volume flow is needed to achieve the same energy input as methane [9]. Therefore, combustors must be adjusted to achieve the required volume flow rates. Another property of H_2 to consider is its flame speed. H_2 has a flame speed that is an order of magnitude faster than other conventional fuels [10]. High flame speed may cause flame instability problems and needs to be adjusted.

These two points prevent the usage of current combustors, designed for typical hydrocarbon flames, to be used for pure H_2 fuels. To use pure H_2 , combustors that are typically intended for H_2 combustion are needed. Moreover, hydrogen's high flammability, low luminosity, and high diffusion can cause some safety problems. A lot more research on pure hydrogen combustion is needed to overcome these difficulties.

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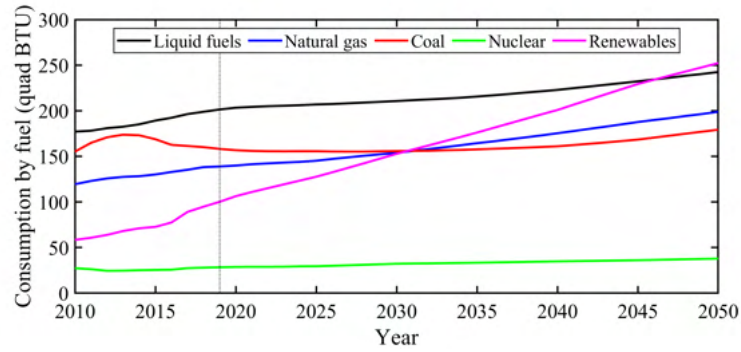


Figure 1.1: Primary energy consumption of the world by fuel. Years after 2019 shows projections. [1]

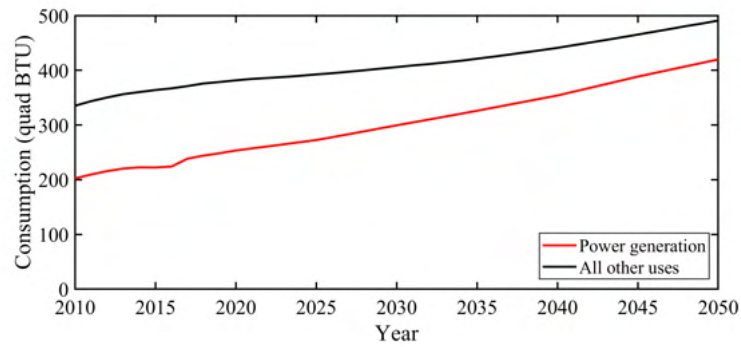


Figure 1.2: Primary energy consumption of the world for power generation and other uses. Years after 2019 shows projections [1]

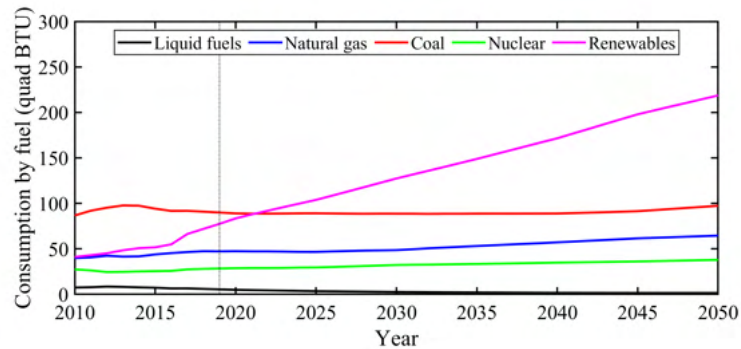


Figure 1.3: Energy consumption of the world by fuel for power generation. Years after 2019 shows projections [1]

1.2 Lifted flames

Combustion systems are categorized under two main categories: premixed systems and non-premixed systems. In premixed systems, fuel and oxidizer are mixed before entering the combustion chamber. In non-premixed systems, fuel and oxidizer are injected into the combustion chamber in different streams and partially mix just before combustion. It is less complicated to build non-premixed and partially premixed systems, and many combustion devices, including gas turbines, operate with non-premixed modes.

Partial mixing of the fuel and oxidizer just before combustion potentially results in three-branched (tribrachial) lifted flames [11]. Here, the incomplete mixing of the fuel and oxidizer leads to a lean premixed flame branch on the oxidizer side and a rich premixed flame branch on the fuel side. The excess reactants that were not consumed by these two branches form a diffusion flame branch. A schematic of this flame structure is given in Fig. 1.4. Under certain conditions, it is also possible that branches collapse, and the structure can become two-branched or single-branched (ordinary diffusion flame) [12]. For fuels with more complex chemical structures, it is even possible that more than three branches are observed [13, 14].

Lifted flames are preferred in the design of many combustion devices

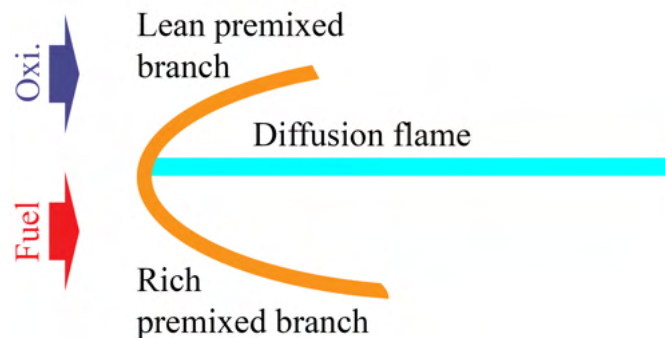


Figure 1.4: A schematic representation of a typical tribrachial flame structure.

due to several reasons. Obtaining lifted flames require high fuel injection velocities that can detach the flame from the fuel nozzle. This allows the size of the injection equipment to be minimized. Moreover, lifted flames allow the fuel and oxidizer to mix partially before the combustion, which reduces the emissions. Another important advantage of lifted flames is that they reduce the heat transfer back to the injection equipment. This allows common metals to be used for the manufacturing of the burners instead of expensive ceramics.

The longer the lift-off height, the more advantageous the lifted flames become. However, if the lift-off height becomes too long, the flame can become unstable or even blow off entirely. Therefore, the stabilization dynamics of lifted flames have been investigated extensively, and several stabilization mechanisms have been suggested. Five of the main ones are: critical scalar dissipation stabilization, premixed flame propagation stabilization, edge-flame stabilization, large-eddy stabilization, and autoignition stabilization [15, 16].

1.2.1 Critical scalar dissipation stabilization

This concept, also named as flamelet extinction model, was proposed by Peters *et al.* [17]. The model suggests that the turbulent flame consists of an ensemble of laminar diffusion flamelets that are highly distorted by the turbulent flow. The scalar dissipation rate is the determining phenomenon of stabilization. When the scalar dissipation rate is over a critical value, the heat dissipation overtakes the chemical reactions. This results in the quenching of the laminar diffusion flamelets, making the critical dissipation rate a marker of lift-off (extinction).

Several studies investigated the role of the scalar dissipation rate on the stabilization of the lifted flames [18, 19, 20, 21, 22, 23]. The main conclusion of these studies is that the role of the critical scalar dissipation rate on flame

stabilization cannot be neglected as it can define the flame base location. However, critical scalar dissipation is not a flame stabilization mechanism on its own.

1.2.2 Premixed flame propagation stabilization

In 1966, Vanquickenborne and van Tiggelen published an article proposing that lifted diffusion flames are stabilized by a balance between the flow velocity and the turbulent burning velocity [24]. Since then, the proposed mechanism was adjusted [25] and supported for flames with long lift-off heights [26]. In addition, this mechanism suggests that the blow-out occurs when the burning velocity is lower than the flow velocity, rather than the flame exceeding the flammability limits [27].

1.2.3 Edge-flame stabilization

The edge-flame stabilization proposes that the flame is supported by the upstream propagation of the partially premixed edge flame along the stoichiometric surface [28]. This mechanism differs from the premixed flame propagation mechanism by its narrow flammable distance up to several laminar-flame thicknesses [16]. Many studies showed that the propagation of laminar edge-flames can be stabilized by the flow velocity [29, 30, 31, 32, 33, 34, 35]. Studies of turbulent lifted flames also showed edge-flame structure [16, 19, 23, 36].

1.2.4 Large-eddy stabilization

Many studies also investigate the role of large-eddies in flame stabilization. The large-eddy stabilization concept is mainly based on the idea that the flame propagates from one eddy to another one in the upstream [37, 38]. Other experimental studies also speculated that the large-eddies affected the lift-off height [39, 40, 41, 42]. However, none of the studies was able to identify the large-eddies as the determining mechanism of flame stabilization.

1.2.5 Autoignition stabilization

Autoignition is another stabilization mechanism that is observed for lifted flames with heated co-flows. Several experimental and numerical studies propose autoignition as the main stabilization mechanism [43, 44, 45, 46, 47].

It is also possible that more than one stabilization mechanism co-exists with each other. Even though it is not yet clear how lifted flames stabilize under certain conditions, recently, it is suggested that autoignition and flame propagation are the main competing mechanisms for lifted flames of moderate lift-off heights [13, 46, 48, 49].

1.3 Numerical studies of turbulent combustion

Combustion is a complex phenomenon that involves turbulence–flame interactions. Therefore, an accurate understanding of combustion requires precise measurements of both thermochemical (i.e., temperature, density, pressure, species concentration) and flow (i.e., velocity field) variables. Experimental and numerical studies of combustion shed light on the combustion phenomena.

There are several experimental methods used to measure the physical quantities in the combustion field. Owing to the technological developments over recent years, laser diagnostic technologies are commonly used to measure field data non-intrusively. Particle image velocimetry (PIV) is one of the optical methods widely used to obtain instantaneous velocity data [36, 50, 51]. However, even though some experimental studies used tomographic particle image velocimetry (TPIV) to capture the three-dimensional (3D) structure of turbulence–flame interactions [52, 53], 3D experimental data is hard to achieve with current laser imaging tools. The most commonly used imaging technology is the laser-induced fluorescence (LIF) technique, which

uses a laser sheet to illuminate the flow field at a wavelength that can excite a target species [42, 43, 54, 55, 56]. Then, the concentration of the species can be captured by the light it emits. However, this spectroscopic method is not only limited to a two-dimensional plane but it is also limited by the repetition rate of the lasers and the capability of detecting other species.

Numerical studies use several numerical approaches to simulate the combustion field by solving the relevant governing equations. There are three main approaches: Reynolds-averaged Navier–Stokes (RANS) approach, large eddy simulation (LES), and direct numerical simulation (DNS).

1.3.1 Reynolds-averaged Navier–Stokes (RANS)

The Reynolds-averaged Navier–Stokes (RANS) approach initially decomposes the instantaneous quantities in the Navier–Stokes equations into their time-averaged and fluctuating quantities and then uses ensemble averaging that results in unclosed terms. These unclosed terms are then modeled using different methods. This approach is widely used for designing combustion devices on an industrial scale, owing to its low computational cost. However, the complex nature of turbulent combustion cannot be accurately analyzed by RANS models. For example, the unsteady phenomena that can affect auto-ignition, stabilization, or extinction cannot be understood in detail by using the averaged quantities of RANS models. Nevertheless, several studies used the RANS approach to model lifted flames [45, 46, 57, 58].

1.3.2 Large-eddy simulation (LES)

The large-eddy simulation uses spatial filtering to the governing equations and ignores the length scales smaller than a user-defined filter size. Since the large length scales are resolved, LES gives more accurate results than RANS models but is more computationally expensive. The smallest length scales removed from the numerical solution by filtering are modeled, and

their effect on the flow field is considered. The accuracy of the LES depends on the accuracy of the models used. LES can capture the unsteady flame and flow phenomena, which RANS models could not. Therefore, LES is a preferred approach to model non-premixed flames [59, 60, 61, 62]. However, it should be noted that LES cannot capture the small-scale turbulence–flame interactions, which results in reduced accuracy.

1.3.3 Direct numerical simulation (DNS)

Direct numerical simulation solves all the relevant governing equations using solely numerical methods, without modeling any terms, and therefore it is the most accurate numerical approach. However, it is also the most computationally expensive method as it needs a high spatial and temporal resolution to resolve the whole range of time and length scales. Its high computational cost prevents it from being used for industrial purposes and limits its usage to simple geometries. The number of DNS studies of lifted turbulent flames is also limited [15, 16, 47, 48, 63, 64] for the same reason. However, its high accuracy and ability to solve unsteady phenomena such as auto-ignition, extinction, and stabilization mechanism make it a useful tool for studying turbulent combustion. DNS results are also used to improve the RANS and LES models.

1.4 Background for DNS research on turbulent combustion of lifted flames

Several studies have investigated turbulent lifted jet flames using three-dimensional (3D) direct numerical simulation (DNS). Mizobuchi *et al.* [63, 64] studied a hydrogen lifted flame in still air. They used the flame index (*FI*) to observe a leading-edge flame possessing triple-flame elements and floating diffusion flame islands downstream. Yoo *et al.* [47] also investigated a hydrogen lifted flame, but their jet was surrounded by heated co-flowing

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air. They did not observe floating flame islands under similar jet Reynolds number conditions to those of Mizobuchi and colleagues. This contrast is possibly caused by the difference in jet exit configuration (round jet versus slot jet) and the existence of autoignition. Yoo *et al.* used statistical analyses to identify a diffusion flame and a rich premixed flame downstream of the flame base, but they found a negligible lean premixed flame.

Karami *et al.* [16] worked with one-step hydrocarbon chemistry and observed a mostly one-branched diffusion flame structure possessing a weak rich premixed flame and no lean premixed flame. Krisman *et al.* [13] reported that in dimethyl ether laminar lifted jet flames, the chemical kinetics of the large hydrocarbon results in a complex, five-branched flame structure. Although they could not physically observe these branches for a corresponding turbulent lifted flame, statistical analyses by Minamoto *et al.* [14] revealed that such branches exist. Dalakoti *et al.* [15] studied a spatially developing n-dodecane round jet flame. The flame showed a three-branched structure at the flame base. Ignition kernels were observed upstream of the flame base. The stabilization mechanism of the flame was analyzed in detail, and it was shown that the flame propagation mechanism stabilizes the flame.

1.5 Objectives of this study

Numerical studies of non-premixed lifted flames mentioned in the previous section considered configurations of single jet flames. However, in many practical gas-turbine combustors, the mixtures are issued from multiple jet exits to enhance mixing, potentially producing multiple lifted-flame bases. Consequently, these flames might interact with one another, resulting in complex flame structures. Some experimental studies of partially premixed turbulent flames used five-slot burners with alternating equivalence ratios to observe the interaction between lifted edge flames [54, 55, 65]. These studies shed light on fundamental combustion features such as the global flame speed and the stabilization mechanisms when these flames interact with one another. However, understanding the flame structure is also essential, especially regarding combustion modeling. For example, turbulent mixing, which results in complex flame structures, should be investigated in 3D physical and phase spaces in detail. DNS would be a valuable tool for such analyses.

Various numerical studies have considered partially premixed turbulent hydrogen flames [47, 63, 64], and increased interest in hydrogen fuel makes these papers relevant today [66]. However, despite the potential relevance, there have been no DNS studies that involve both steam dilution to further decrease the emissions and a multi-jet configuration, to the best of the present author's knowledge. Therefore, in this study, the flame features of lifted jet flames of non-premixed hydrogen and steam-diluted oxygen are investigated using DNSs.

The first objective of this study is to identify if steam dilution results in a change in the structure or stabilization mechanism of the lifted jet flames. The second objective is to determine if the pressure affects the flame structure or stabilization mechanism under nominal gas turbine thermochemical conditions. This is needed to verify the usage of moderate pressure in the turbulent DNS study. The third objective is to investigate the effect of multi-

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jets on the structure and stabilization of lifted flames without the influence of turbulence. The fourth objective is to identify the flame structure and stabilization mechanism of turbulent lifted multi-jet flames under nominal gas turbine conditions.

For these purposes, the remainder of this dissertation is organized as follows. In the first part of Ch. 2, the effect of steam dilution on the flame features of lifted flames of H_2 and O_2 is investigated using DNS of canonical laminar half-jet configurations. The structure and stabilization mechanism of steam diluted flames are investigated and compared with the nitrogen diluted flames under the same thermo-chemical conditions. Another parameter to be investigated is the effect of pressure on the flame features. Since the high computational cost limits the DNS of 3D turbulent combustion studies to moderate pressures, investigating the pressure effects is essential. Therefore, in Sec. 2.6, the effect of steam dilution and pressure on the ignition characteristics are investigated simultaneously, using the homogeneous gas reactor module of CHEMKIN-PRO. Then, the effect of pressure on the flame features of the lifted flames under nominal gas turbine conditions is investigated using canonical DNS configurations similar to the first part of Ch. 2.

In Chs. 3 and 4, features of multi-jet lifted flames under the nominal gas turbine conditions are investigated. The main objective is to discover whether the flames interact with one another and, if they do, to investigate the effect of these interactions on the flame structure. In Ch. 3, DNSs of two-dimensional laminar flames are performed to reveal the fundamental features of multi-jet lifted flames, without the influence of turbulence, and finally, in Ch.4, a 3D turbulent case, with the same thermochemical conditions as in the laminar cases, is investigated.

Chapter 2

Laminar non-premixed lifted flames of H_2 and O_2 diluted with steam

2.1 Preface

The structure and stabilization mechanism of lifted flames highly depend on the thermo-chemical conditions. As mentioned previously in Sec. 1.2, branches of typical tribrachial flames may collapse, or more than three branches may be observed for different fuels with complex chemical behaviors.

This study uses steam (H_2O) as the oxidizer diluent instead of the conventional diluent, nitrogen (N_2). H_2O prevents NO_x emissions, but it has different chemical and physical properties compared with N_2 . Therefore, it is essential to investigate the effect of steam on the flame structure and stabilization mechanism.

Another factor that may affect the fundamental flame features is the pressure. Higher pressures result in thinner flames, which require higher resolution for numerical studies. However, the computational cost of DNS, especially in 3D space, prevents the use of high pressures, whereas practical gas turbines work with high compression ratios. The final chapter of this thesis is an example of such a DNS study, where the flame features of turbu-

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lent multi-jet flames are investigated under nominal gas turbine conditions. However, a moderate pressure of 2 atm is used due to such a configuration's expensive computational cost. Since pressure is another determining factor on flame features, it is necessary to examine the effect of pressure on the flame structure and stabilization under nominal gas turbine conditions.

The effect of diluent and pressure on the fundamental flame features are investigated in this chapter as follows. In Sec. 2.2, the numerical methods used in DNS are summarized. Domain configurations used for DNS are explained in Sec. 2.3. The flame structure of H_2O diluted case in comparison to N_2 diluted case is shown in Sec. 2.4, and the flame stabilization mechanisms of these cases are explained in Sec. 2.5. In Sec. 2.6, the effect of steam dilution and pressure on the ignition delay time is investigated using the homogeneous gas reactor module of CHEMKIN-PRO. In Secs. 2.7 and 2.8, the effect of pressure on the flame structure and flame stabilization mechanism is investigated using laminar lifted flame configurations similar to Secs. 2.4 and 2.5. Four different pressure cases varying from 2-20 atm are investigated. Finally, the findings are concluded in Sec. 2.9.

2.2 Numerical methods

DNSs are conducted using a solver, TTX, developed at the Tokyo Institute of Technology [67]. This program solves fully compressible conservation equations for the mass, momentum, energy, and mass fraction of $N_s - 1$ species, considering temperature-dependent transport and thermal properties. Here, N_s is the total number of species involved in combustion. The equations are discretized on a uniform Cartesian mesh using a fourth-order central finite difference scheme and integrated in time using a third-order Runge–Kutta scheme. In addition, the multi-timescale (MTS) solver [68] with the correlated dynamic adaptive chemistry and transport (CO-DACT) method [69, 70] is adopted for the time integration of chemical source terms to increase the computational speed. Finally, a detailed chemical-kinetic mechanism for hydrogen combustion with nine reactive species and 21 elementary reactions is used [71]. A detailed explanation of the governing equations solved, as well as the numerical methods used for DNS, can be found in Appendix A, and the description of the chemical kinetic mechanism is given in Appendix B.

2.3 Domain configurations

In this chapter, the effects of diluent type and pressure on the flame features are investigated using two-dimensional (2D) half-burner configurations. Previous studies used similar configurations to investigate 2D lifted flames [13, 72]. The domains are configured as rectangles that have adiabatic free slip boundary conditions in transverse directions. The fuel is fed to the domain from the upper half of the inlet boundary at $x = 0$, and the oxidizer is fed from the lower half of the same boundary. The boundary at $x = L_x$ is set as an outflow boundary. All of the boundaries are specified using Navier–Stokes characteristic boundary conditions (NSCBC) [73].

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Table 2.1: Domain parameters and thermochemical conditions for the comparative study of H₂O and N₂ dilutions

	S-H2O	S-N2
$L_x \times L_y$ (mm)	25.00×15.00	25.00×15.00
$N_x \times N_y$	1440×896	1440×896
δt (ns)	2.0	2.0
Pressure (atm)	1.0	1.0
Fuel	H ₂	H ₂
Oxidizer (by mole)	0.12 O ₂	0.12 O ₂
	0.88 H ₂ O	0.88 N ₂
T_f (K)	400	400
T_{oxi} (K)	900	900

In the first section of this chapter (Sec. 2.4), the effect of H₂O dilution is investigated compared to N₂. The H₂O diluted case is named S-H2O, and N₂ diluted case is named S-N2. Both cases have domain sizes of $L_x \times L_y = 25.00 \times 15.00$ mm² and the domains are discretized by $N_x \times N_y = 1440 \times 896$ uniform mesh points. The fuel is pure H₂ at 400 K. The oxidizer stream at 900 K consists of 12% O₂ by mole, and the remainder of the stream is diluted either by H₂O or N₂. The pressure is set to 1 atm, and the initial inflow velocity is set to 10 m/s at $x = 0$ for both cases. The inflow velocity is adjusted to maintain the flame base at a certain position. After the solution reaches a steady-state, the final inflow velocity is 9.56 m/s and 13.02 m/s for S-H2O and S-N2, respectively. Thermochemical conditions and domain parameters are summarized in Table 2.1.

The following tangential profile specifies the scalar profiles at the inlet:

$$q_{in} = q_c + \frac{q_j - q_c}{2} \left[\tanh \left(\frac{y}{2\delta} \right) + 1 \right], \quad (2.1)$$

where the generic quantity q corresponds to the scalars, such as temperature and mass fractions of H₂, O₂, and H₂O. The subscripts j and c correspond to the fuel jet and oxidizer co-flow, respectively.

In the second part of this chapter (Sec. 2.7), the effect of pressure on the

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Table 2.2: Domain parameters and thermochemical conditions for the parametric study of pressure under practical gas turbine conditions.

Pressure (atm)	2.0	4.0	10.0	20.0
$L_x \times L_y$ (mm)	12.50×7.50	12.50×7.50	8.00×4.80	8.00×4.80
$N_x \times N_y$	1008×616	3600×2240	3600×2240	7200×4480
δt (ns)	2.500	0.700	0.450	0.225
Fuel	H ₂	H ₂	H ₂	H ₂
Oxidizer (by mole)	0.12 O ₂	0.12 O ₂	0.12 O ₂	0.12 O ₂
	0.88 H ₂ O	0.88 H ₂ O	0.88 H ₂ O	0.88 H ₂ O
T_f (K)	288	288	288	288
T_{oxi} (K)	916.5	916.5	916.5	916.5

flame features is investigated. Except for the pressure, the thermochemical conditions correspond to those of a next-generation hydrogen gas-turbine engine, which has a thermal efficiency of 75% [74]. The domain boundaries are set similar to S-H₂O and S-N₂, and Eq. 2.1 is used to specify the inflow scalar profiles. Since the flame thickness decreases with increasing pressure, the size and resolution of the domains are adjusted accordingly. Four different pressures varying between 2 to 20 atm are investigated, and the thermochemical conditions and domain parameters are summarized in Table 2.2.

2.4 Effect of steam dilution on the flame structure

Figure 2.1 shows the temperature (T), logarithmic heat-release rate ($\dot{Q}$), and normalized flame index (NFI) distributions of the H₂O diluted case (S-H₂O) and N₂ diluted case (S-N₂) for regions with a substantial heat-release rate, $\dot{Q} > 0.01\dot{Q}_{max}$. The contours are superimposed with dashed and dotted lines. The dashed lines show the iso-lines of OH mass fraction corresponding to 5% of its maximum value ($Y_{OH} = Y_{OH,5\%}$), and the dotted lines correspond to the stoichiometric mixture fraction (ξ_{st}) iso-lines in each domain. ξ_{st} values of S-H₂O and S-N₂ are 0.025 and 0.017, respectively.

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The definition of the mixture fraction (ξ), based on Ref. [75], is as follows:

$$\xi = \frac{\frac{1}{2}(Z_H - Z_{H,o})/W_H - (Z_O - Z_{O,o})/W_O}{\frac{1}{2}(Z_{H,f} - Z_{H,o})/W_H - (Z_{O,f} - Z_{O,o})/W_O}, \quad (2.2)$$

where Z_H and Z_O represent the elemental mass fractions, and W_H and W_O represent the molecular weights of hydrogen and oxygen atoms, respectively. The subscripts f and o correspond to the fuel and oxidizer streams, respectively.

A Y_{OH} or OH image is used as a flame-base marker in experimental and numerical studies [42, 43, 47, 51, 61, 76]. Therefore, it is reasonable to define the flame-base position based on the most-upstream position of the $Y_{OH} = Y_{OH,5\%}$ iso-lines, enclosing the regions with a high heat-release rate. However, in this study, as described in detail in Sec. 4.3, the flame-base position is defined as the location of the intersection between the $Y_{OH} = Y_{OH,5\%}$ and $\xi = \xi_{st}$ iso-lines (surfaces). Such positions can be clearly seen in the laminar flame results. Moreover, the conventional definition of the flame-base position—the most-upstream position of the $Y_{OH} = Y_{OH,5\%}$ surface [47, 61, 76]—is close to the present flame-base position, as seen in Fig. 2.1.

Figures 2.1a and 2.1b show the temperature distributions of both cases. It is seen that the S-N₂ case has higher temperatures than the S-H₂O case, especially around the ξ_{st} iso-line. This results from the high heat capacity of steam, and it is an essential difference as it may result in a change in the structure or stabilization mechanism of the flame.

Figures 2.1c and 2.1d illustrate the logarithmic $\dot{Q}$ contours. Both cases show similar $\dot{Q}$ distributions. The highest $\dot{Q}$ values are observed around the flame base, slightly towards the rich mixtures ($\xi > \xi_{st}$). Based on the $\dot{Q}$ distributions, the lean premixed and diffusion flame branches of the flames in both cases cannot be distinguished from each other. This feature is caused by the high diffusivity of H₂, which shifts ξ_{st} towards the lean side ($\xi < \xi_{st}$). A similar effect of hydrogen diffusivity on the flame structure was previously observed by Im *et al.* [77].

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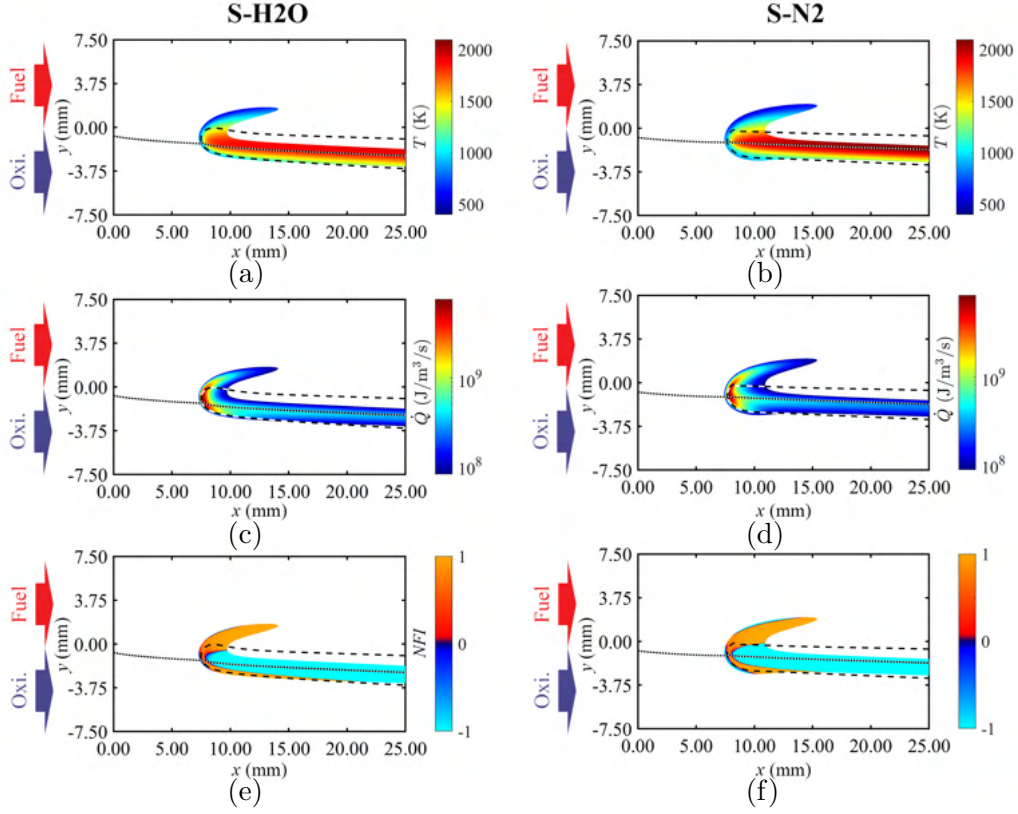


Figure 2.1: (a,b) Temperature (T), (c,d) logarithmic heat-release rate ($\dot{Q}$), and (e,f) normalized flame index (NFI) for (a,c,e) S-H₂O, and (b,d,f) S-N₂. Contours are shown for regions with a substantial heat-release rate, $\dot{Q} > 0.01\dot{Q}_{max}$. The dashed and dotted lines correspond to $Y_{OH} = Y_{OH,5\%}$ and ξ_{st} iso-lines, respectively.

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The flame index is computed to show the mixing structure. This parameter has been widely used [47, 63, 64, 66, 78] since it was first defined in Ref. [79] to investigate the mixing mode of the combustion field. The present study uses the normalized flame index (NFI), defined as the following in Ref. [47]:

$$NFI = \frac{\nabla Y_f \cdot \nabla Y_o}{|\nabla Y_f| |\nabla Y_o|}. \quad (2.3)$$

As can be understood from this equation, the NFI gives the cosine of the angle between the fuel (f) and oxidizer (o) gradients. Thus, positive NFI values represent the premixed mode, whereas negative values correspond to the non-premixed mode.

Figures 2.1e and 2.1f reveal the typical tribrachial structure for both cases. The premixed flame branches are observed on lean and rich sides, and the diffusion flames trail along the ξ_{st} iso-lines. The high diffusivity of H_2 , discussed above, shifts the position of the diffusion flames towards the lean side along with the ξ_{st} iso-lines, leading to the collision of the diffusion and lean premixed flames. Nevertheless, the flame index clearly shows the presence of three flame branches.

Conditional averages of $\dot{Q}$, T , and the NFI on ξ , as well as the probability density function (PDF) of ξ , for the regions with a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) are illustrated in Fig. 2.2 for cases S-H₂O and S-N₂. PDF and NFI distributions of both cases (Figs. 2.2a and 2.2b) show similar behaviors. Both cases have a peak in the PDF at $\xi \approx \xi_{st}$, which corresponds to the diffusion flame branch, as can be seen by the negative NFI values in Fig. 2.2b. Moreover, there are no peaks on the lean or rich side for both cases, reflecting the relatively small volume of lean and rich flame branches compared with the volume of diffusion flame. The positive NFI values on the lean and rich sides for both cases suggest the existence of lean premixed and rich premixed flame branches, revealing the typical tribrachial flame structure of a non-premixed lifted flame together with a diffusion flame branch.

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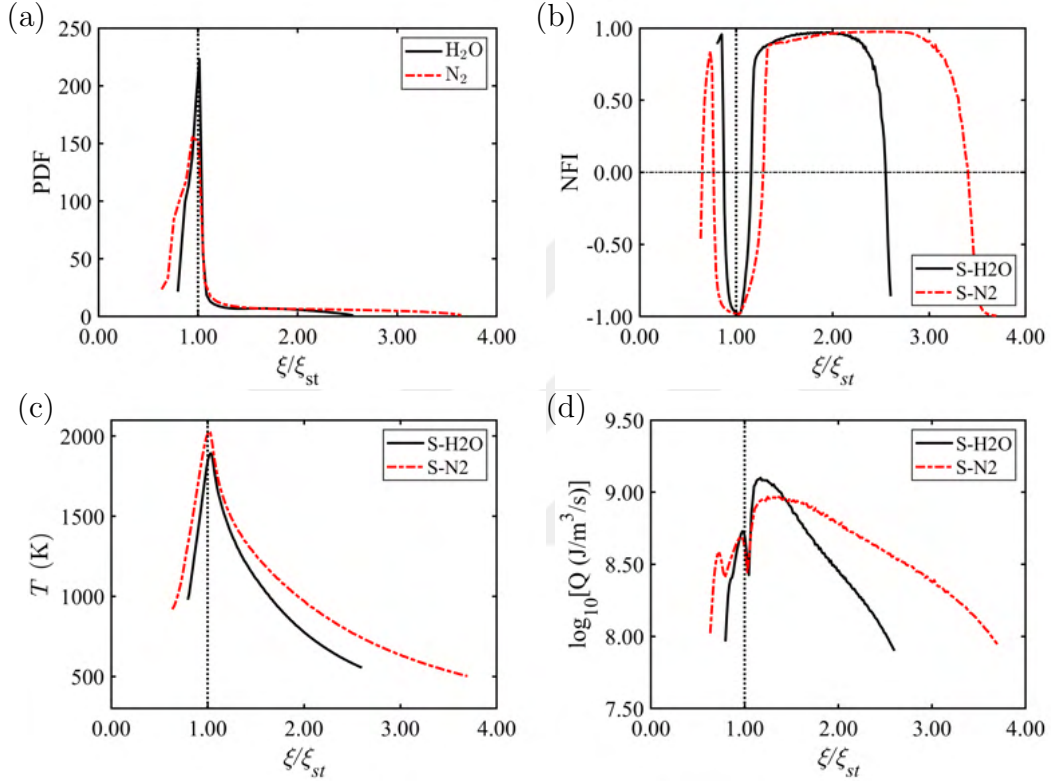


Figure 2.2: PDF of mixture fraction (ξ) (a), and average values of the normalized flame index (NFI) (b), temperature (T) (c), and heat-release rate ($\dot{Q}$) (d) conditioned on ξ for the S-H₂O and S-N₂ cases. ξ values are normalized by the ξ_{st} of each case. The vertical lines correspond to $\xi_{st} = \xi_{st}$. Only samples that have substantial $\dot{Q}$ values ($\dot{Q} > 0.01\dot{Q}_{max}$) are used.

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Figure 2.2c shows the mean temperature of both cases, conditioned on ξ . Both cases follow a similar trend in the ξ phase space in the sense that there is a peak observed at ξ_{st} . S-H₂O has lower T values than S-N₂ on average because of the high heat capacity of steam, which decreases the overall temperature.

Figure 2.2d illustrates the average $\dot{Q}$ conditioned on ξ . S-H₂O shows two peaks, the first one around ξ_{st} , and the second in slightly rich regions. The peak in the rich regions is higher than the first one. This first peak observed around stoichiometry corresponds to the collapsed branches of diffusion and lean premixed flames, as can be seen from the NFI values in Fig. 2.2b. For the S-N₂ case, on the other hand, three peaks that correspond to lean premixed, diffusion, and rich premixed flames, respectively, are observed in Fig. 2.2d. These three $\dot{Q}$ peaks were not apparent in the $\dot{Q}$ contours shown in Fig. 2.1d. This difference between the mean $\dot{Q}$ plots of S-H₂O and S-N₂ suggests that the two cases may have different chemical reactions and species distributions.

Figure 2.3 shows the mass fraction contours of certain species for both of the cases. Qualitatively, the species mass fractions of both cases show similar distributions except for the HO_2 . For the S-H₂O case, Y_{HO_2} is high on both the lean and rich sides, whereas for the S-N₂ case, Y_{HO_2} is concentrated on the rich side. To compare the mass fractions of the species in both cases quantitatively and to investigate the effect of steam dilution on the chemical reactions, the mass fractions of certain species and reaction rates along the ξ iso-lines at stoichiometry, as well as the lean and rich sides are shown in Figs. 2.4-2.9. The lean mixture fraction iso-line corresponds to $\xi \sim 0.8\xi_{st}$, the rich mixture fraction iso-line corresponds to $\xi \sim 1.2\xi_{st}$ for both cases, and they are shown with dotted lines in Fig. 2.3, as well as the ξ_{st} iso-line.

Figures 2.4a and 2.4b show the mass fractions of certain species along the lean ξ iso-line for S-H₂O and S-N₂ cases, respectively. The mass fraction values are normalized by the mass fraction value of the species with the

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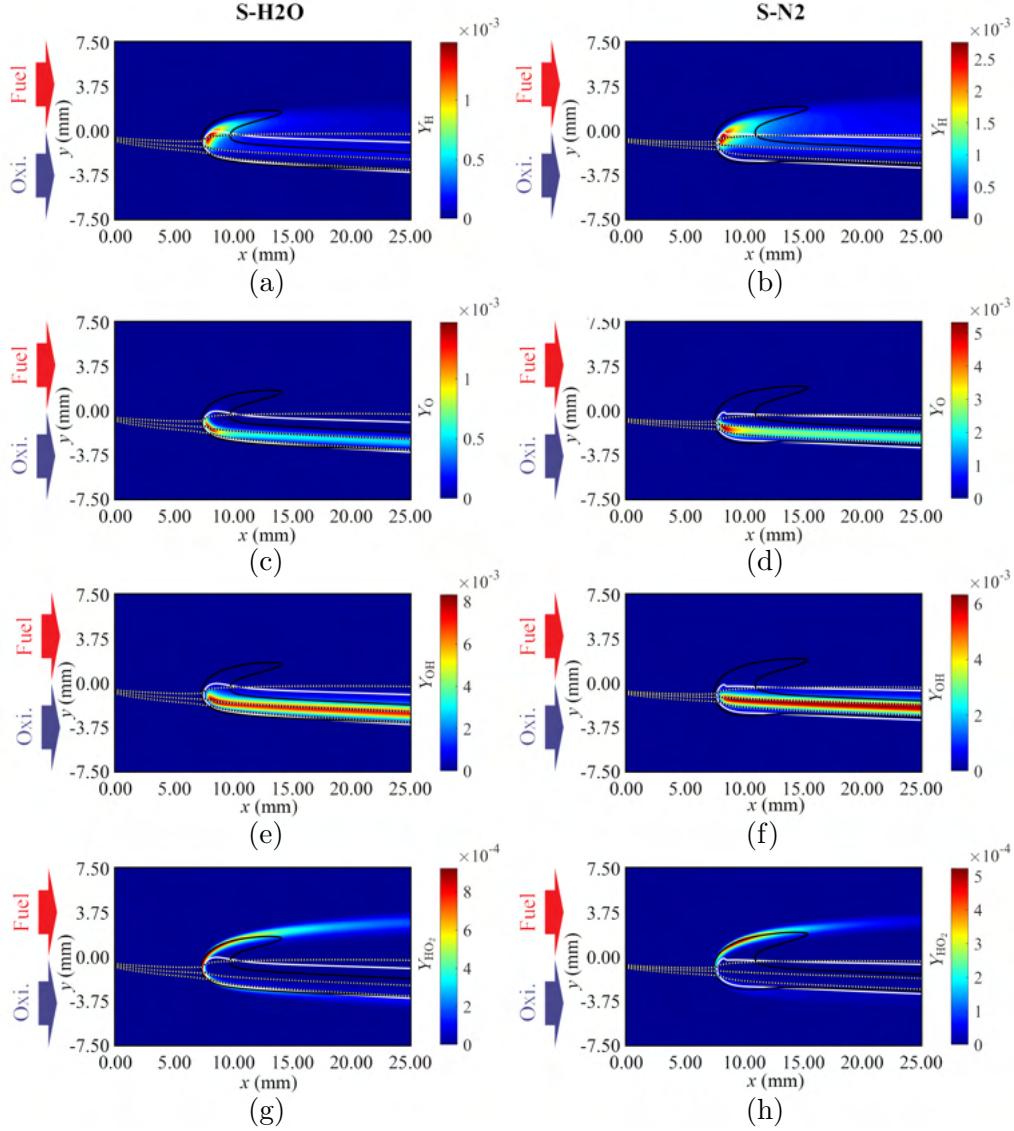


Figure 2.3: (a,b) Temperature (T), (c,d) logarithmic heat-release rate ($\dot{Q}$), and (e,f) normalized flame index (NFI) for (a,c,e) S-H₂O, and (b,d,f) S-N₂. Contours are shown for regions with a substantial heat-release rate, $\dot{Q} > 0.01\dot{Q}_{max}$. The dashed and dotted lines correspond to $Y_{OH} = Y_{OH,5\%}$ and ξ_{st} iso-lines, respectively.

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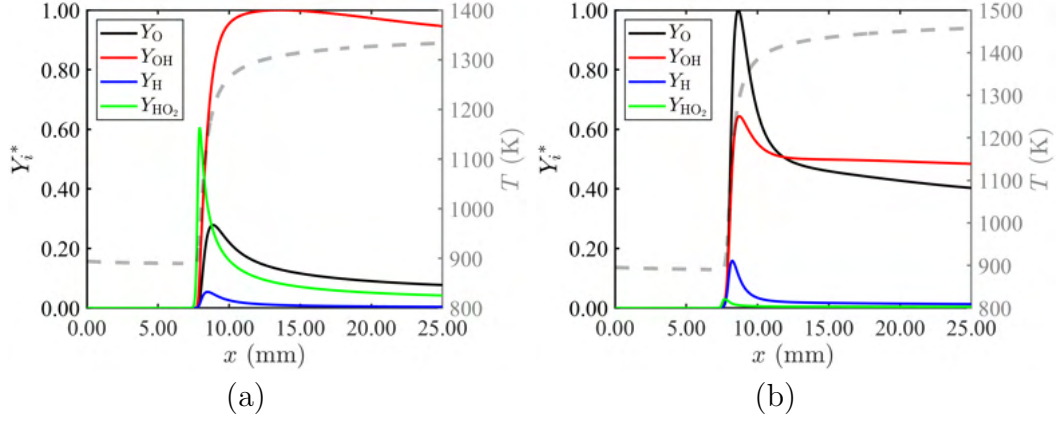


Figure 2.4: Mass fractions of certain species along $\xi \sim 0.8\xi_{st}$ for cases S-H2O (a) and S-N2 (b). The mass fractions are normalized by the mass fraction of the species having the highest Y value along the specified iso-line. The temperature distribution is also shown with a dashed line.

highest Y value along the specified iso-line. For the S-H2O case, OH has the highest mass fraction, while Y_O is the highest for the S-N2 case. Another important difference between the two cases is observed for the Y_{HO_2} distributions. HO_2 has the second highest mass fraction value after OH for the S-H2O case, while it shows the lowest mass fraction values for S-N2.

To investigate the reason behind the different mass fraction values along the lean ξ iso-lines of each case, rate of each reaction along the same iso-line is calculated, and the ones with significant rates are plotted in Fig. 2.5. The reaction rates are normalized by the fastest reaction rate along the $\xi \sim 0.8\xi_{st}$ iso-line for each case. Mentioned reactions can be found in Table 2.3. First reaction to be mentioned is R4. This is a H₂/O₂ chain reaction that produces OH. For the S-H2O case, the net rate of this reaction is positive whereas for the S-N2 case, the net reaction rate is negative, indicating that OH is consumed by this reaction on the lean side of the S-N2. The reason for this difference is the H₂O. As the forward reaction of R4 consumes H₂O, the steam in the oxidizer for the S-H2O case increases the forward rate of this reaction, resulting in an overall net positive reaction rate, which in turn, increases the

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Table 2.3: Chemical reactions mentioned for reaction rate analyses of S-H₂O and S-N₂.

R1	$\text{H} + \text{O}_2 = \text{O} + \text{OH}$
R2	$\text{O} + \text{H}_2 = \text{H} + \text{OH}$
R3	$\text{H}_2 + \text{OH} = \text{H}_2\text{O} + \text{H}$
R4	$\text{O} + \text{H}_2\text{O} = 2\text{OH}$
R9	$\text{H} + \text{O}_2 (+\text{M}) = \text{HO}_2 (+\text{M})$
R10	$\text{HO}_2 + \text{H} = \text{H}_2 + \text{O}_2$
R11	$\text{HO}_2 + \text{H} = 2\text{OH}$
R12	$\text{HO}_2 + \text{O} = \text{OH} + \text{O}_2$
R13	$\text{HO}_2 + \text{OH} = \text{H}_2\text{O} + \text{O}_2$

OH production rate in comparison to S-N₂ case. On the other hand, the reverse reaction rate of R4 for S-N₂ increases the mass fraction of O. The different reaction rates of R4 for both cases can be one of the reasons why the highest mass fraction for S-H₂O case belongs to OH, and O for S-N₂ case.

Another important difference is observed for R9. As can be seen from Fig. 2.5b, R1 is the fastest reaction on the lean side of the S-N₂ case, followed by R2 and then R9. On the other hand, for S-H₂O (Fig. 2.5a), R9 is the fastest, followed by R11, and then R1, which is only as fast as 40% of R9. R9 is a fall-off reaction, and its rate is determined by the efficiency factor of a third body. For the S-H₂O case, this third body is H₂O and for S-N₂, it is N₂. As can be seen in App. B, the efficiency factor of H₂O is 11-12 times higher than that of N₂, which can explain the high reaction rate of R9. Since R9 is a HO₂ production reaction, the high rate of R9 for the S-H₂O also explains the high mass fraction of HO₂ in S-H₂O case, as observed in Fig. 2.4a. The high efficiency factor of H₂O increases the rate of R9 so much that its rate becomes twice the rate of R1 for S-H₂O case, whereas for S-N₂, R9 is 80% as fast as R1. This difference in the rate of R1 results in O mass fraction for the S-H₂O case to be lower than OH and HO₂.

Figures 2.6a and 2.6b show the mass fractions of certain species along

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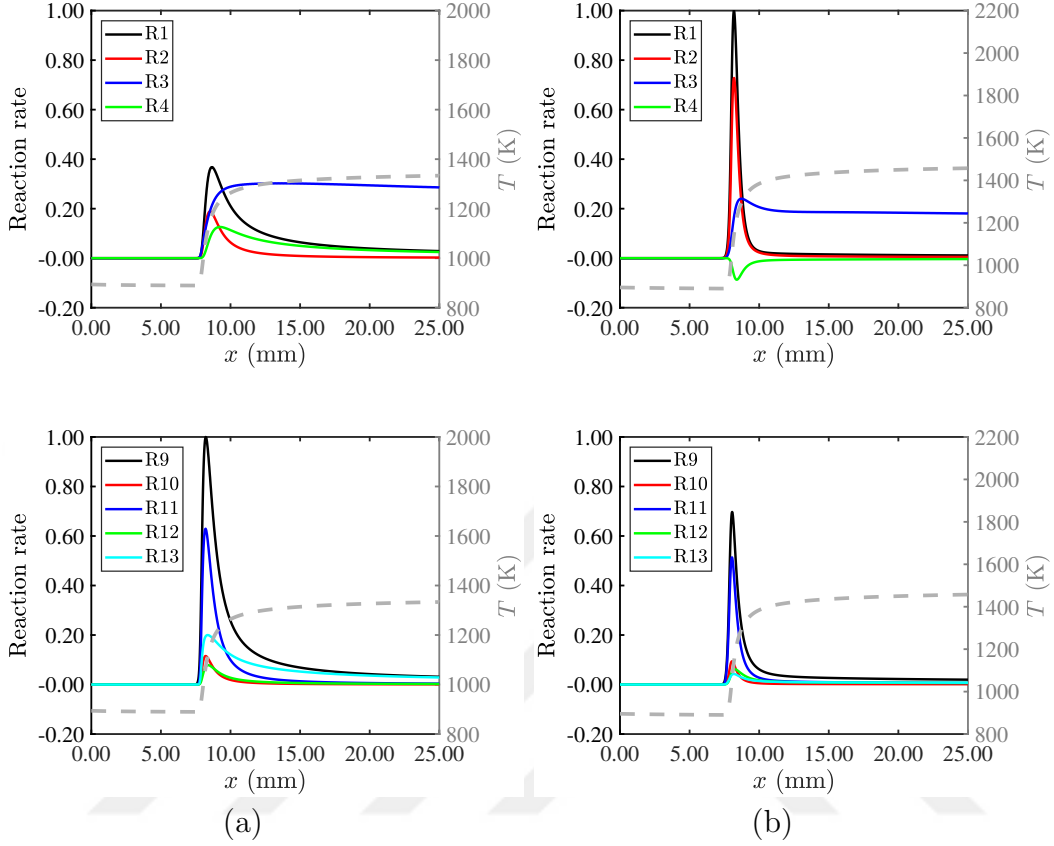


Figure 2.5: Rates of reactions with significant reaction rates along $\xi \sim 0.8\xi_{st}$ for the S-H₂O (a) and S-N₂ (b) cases. The reaction rates are normalized by the fastest reaction rate along the specified iso-line. The temperature distribution is also shown with a dashed line.

the ξ_{st} iso-line for S-H₂O and S-N₂ cases, respectively. On the ξ_{st} iso-line, OH has the highest mass fraction for both cases, and it is followed by O. However, even though O has the second-highest mass fraction in both cases, its value in the S-H₂O case is only 20% of Y_{OH} , while Y_O for S-N₂ is 80% of Y_{OH} . Another important difference between the two cases is observed for the Y_{HO_2} . For the S-H₂O case, HO_2 has the third-highest mass fraction value, even though its value is low, relative to Y_{OH} . On the other hand, Y_{HO_2} value for the S-N₂ is insignificant compared to other species.

To understand the reason behind the different relative mass fraction of

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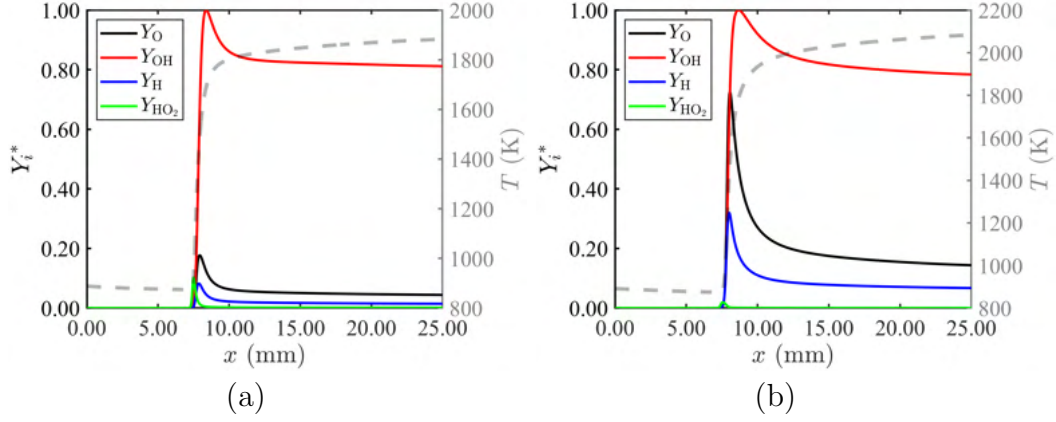


Figure 2.6: Mass fractions of certain species along ξ_{st} iso-line for cases S-H2O (a) and S-N2 (b). The mass fractions are normalized by the mass fraction of the species having the highest Y value along the specified iso-line. The temperature distribution is also shown with a dashed line.

species between two cases, rate of each reaction along ξ_{st} is calculated and the ones with significant reaction rates are plotted in Fig. 2.7. Among the first four reactions, the most significant difference is observed for R4. Its reaction rate is around 30% of the highest reaction rate in S-H2O, whereas it is insignificant for the S-N2 case. This difference results from the H₂O dilution of S-H2O, which increases the forward reaction rate of R4. This increase also contributes to an increase in the Y_{OH} . Another significant difference between the two cases is observed for the reaction rates of R9 and R11. For the S-H2O case, these two reactions are as 60-80% fast as R1, whereas for the S-N2 case, they are only about 30% as fast as R1. This difference in the reaction rates of R9 and R11 is a possible result of high efficiency factor of H₂O, which increases the rate of the fall-off reaction R9. This increase in the rate of R9 results in an increase in Y_{HO_2} , as seen in Fig. 2.6, and the increase in Y_{OH} increases the rate of R11, which increases Y_{OH} even further, and decreases Y_H .

Figures 2.8a and 2.8b show the mass fractions of certain species along $\xi \sim 1.2\xi_{st}$ iso-line for S-H2O and S-N2 cases, respectively. The most significant

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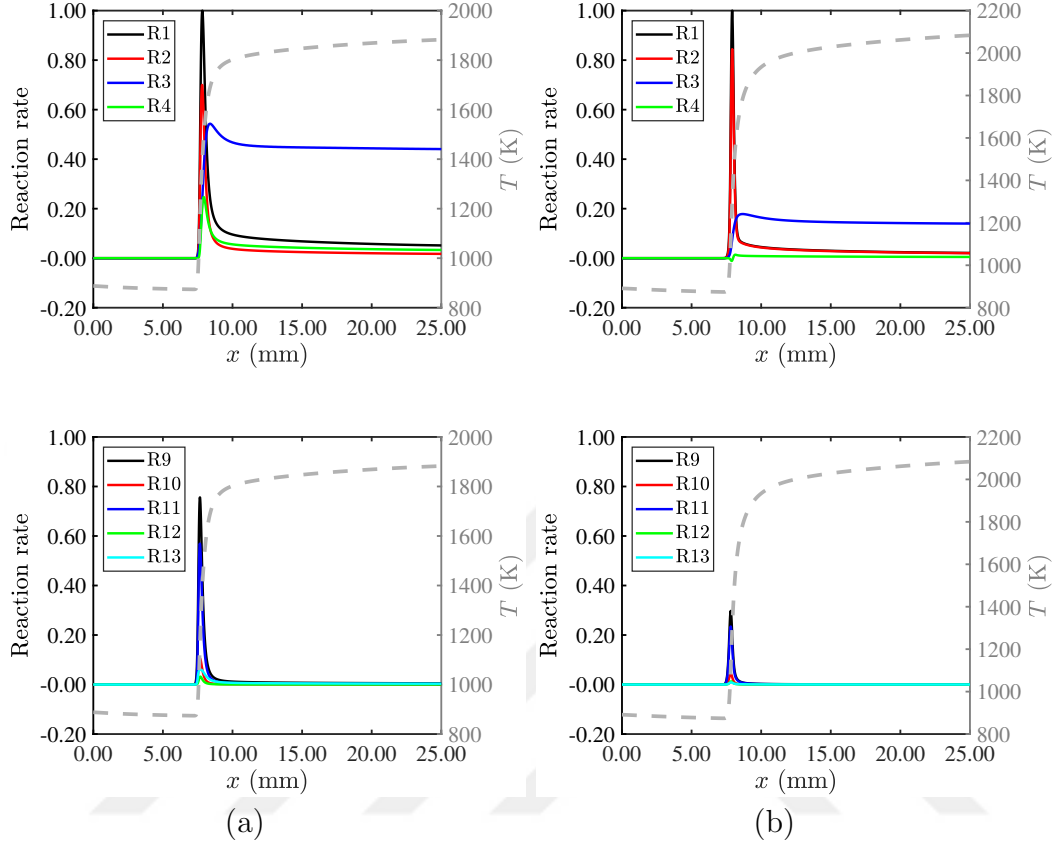


Figure 2.7: Rates of reactions with significant reaction rates along ξ_{st} iso-line for the S-H₂O (a) and S-N₂ (b) cases. The reaction rates are normalized by the fastest reaction rate along the specified iso-line. The temperature distribution is also shown with a dashed line.

difference in the mass fractions is observed for OH and HO₂ between the two cases. For S-H₂O, OH has the highest mass fraction value, whereas for S-N₂, Y_{OH} is only about 40% of Y_O , the highest mass fraction value. As for HO₂, it has the third-highest mixture fraction value for the S-H₂O case, reaching almost 60% of the highest mixture fraction, whereas, for the S-N₂ case, its value is insignificant. Similar to lean and stoichiometric mixture fractions, the reaction rates along the rich mixture fraction iso-line are calculated and presented in Fig. 2.9.

Figure 2.9 shows that the most significant difference in the reaction rates

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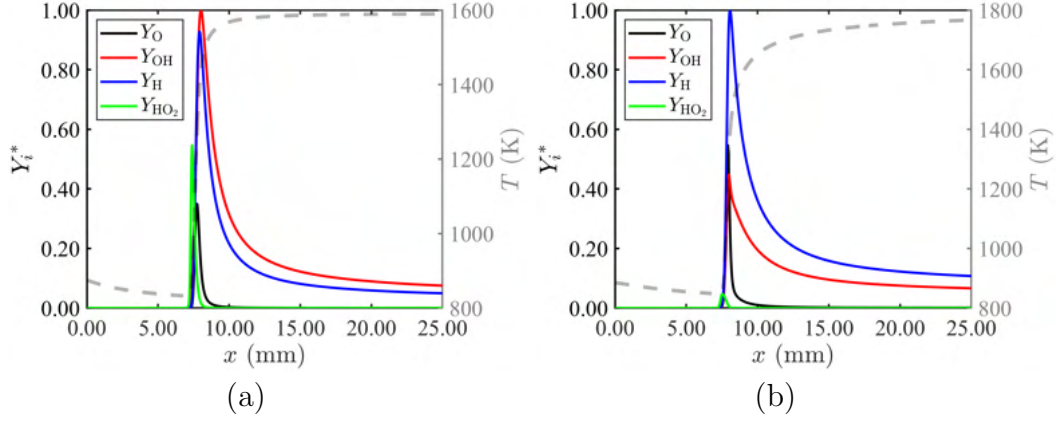


Figure 2.8: Mass fractions of certain species along $\xi \sim 1.2\xi_{st}$ iso-line for cases S-H₂O (a) and S-N₂ (b). The mass fractions are normalized by the mass fraction of the species having the highest Y value along the specified iso-line. The temperature distribution is also shown with a dashed line.

between two cases is observed for reactions R9 and R11. For S-H₂O case, R9 and R11 compete with the fastest reactions, R1 and R2, whereas for S-N₂, they are only as 40% fast as R1 and R2. Similar to the lean and stoichiometric mixture fraction iso-lines, this difference suggests that the high efficiency factor of steam in the S-H₂O case increases R9, which in turn increases R11 through HO₂ production. This difference explains the high Y_{HO_2} observed in Fig. 2.8a. Increase in the reaction rate of R11 increases the Y_{OH} , which results in OH having the highest mass fraction value in Fig. 2.8a.

The species mass fraction and reaction rates along lean, stoichiometric, and rich mixture fraction iso-lines suggest that steam dilution affects the rates of certain reactions, altering the species distributions. This change does not significantly affect the overall flame structure, but it can affect the main stabilization mechanism.

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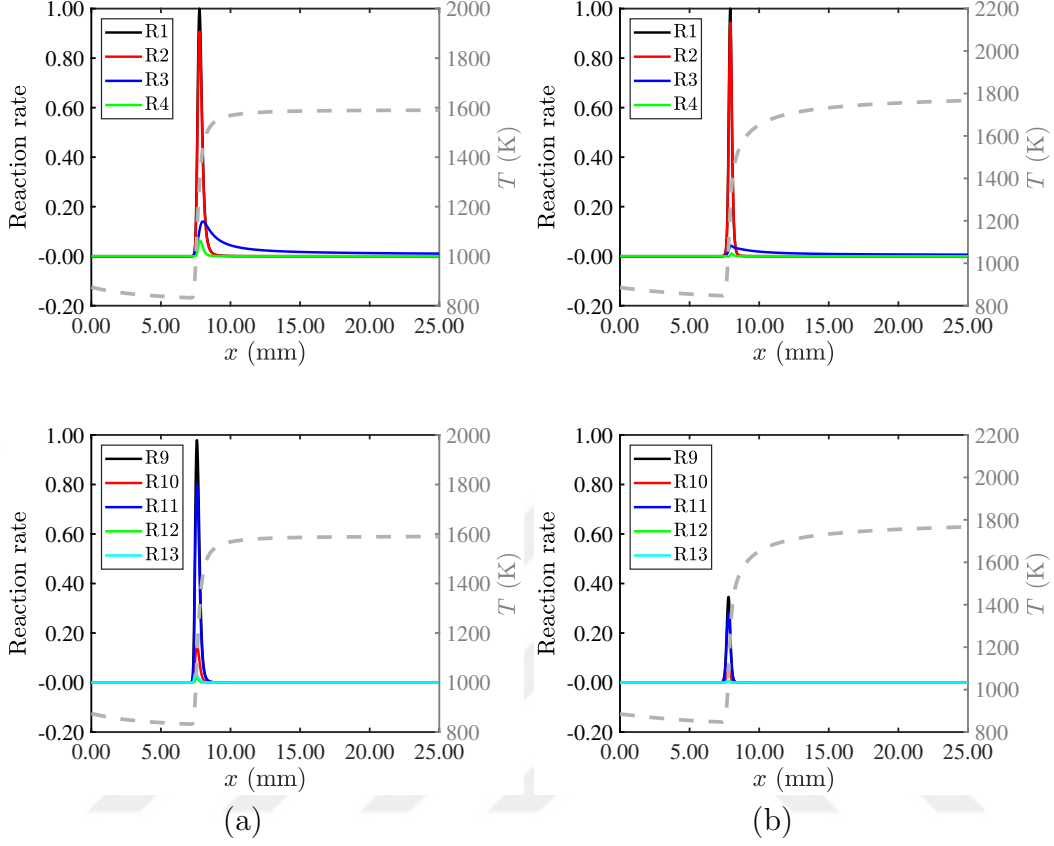


Figure 2.9: Rates of reactions with significant reaction rates along $\xi \sim 1.2\xi_{st}$ iso-line for the S-H₂O (a) and S-N₂ (b) cases. The reaction rates are normalized by the fastest reaction rate along the specified iso-line. The temperature distribution is also shown with a dashed line.

2.5 Effect of steam dilution on the flame stabilization

Transport budget of convection, diffusion, and reaction terms can be used to distinguish the propagation stabilized flames from autoignition stabilized flames, and therefore used by several studies [13, 15, 16, 45, 46, 80, 81]. CDR budget considers the transport equation, given in Eq. 2.4, for a thermochemical variable of interest (e.g. for a species mass fraction, Y_i).

$$\frac{\partial}{\partial t}[\rho Y_i] = -\frac{\partial}{\partial x_j}[\rho Y_i u_j] - \frac{\partial}{\partial x_j}[\rho Y_i V_{j,i}] + \omega_i \quad (2.4)$$

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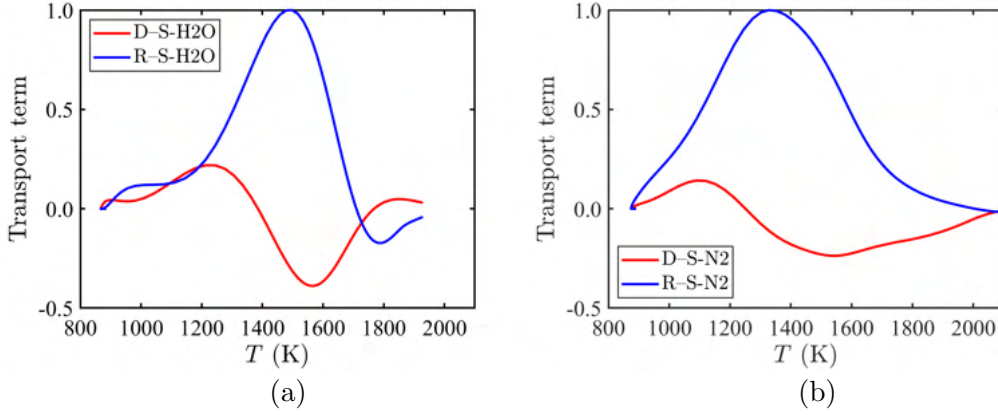


Figure 2.10: Transport budgets of Y_{OH} along the ξ_{st} for cases (a) S-H₂O and (b) S-N₂. The transport terms are normalized by the maximum value of the R-term for both cases.

ρ and $V_{j,i}$ correspond to density and diffusion velocity, and the terms on the right-hand side are convection (C), diffusion (D), and chemical reaction (R) terms, respectively. The left-hand side of Eq. 2.4 is zero for a steady-state solution, and therefore $C + D + R$ terms on the right-hand side should be equal to zero. Diffusion plays an essential role in propagating flames by transporting heat and radicals upstream of the reaction zones. Transported scalars accelerate the combustion in the upstream regions, giving the flame the ability to propagate. Therefore, D and R terms have the same order of magnitude for propagation stabilized flames. For an autoignition stabilized flame, the R term is the dominant one.

OH is one of the major species in hydrogen combustion, and its concentration is also used to define the flame base position, as explained previously. Therefore, in this study, the transport budget of Y_{OH} is used to investigate the flame stabilization mechanism. Figure 2.10 shows the transport budget of Y_{OH} along the ξ_{st} of cases S-H₂O and S-N₂. The transport terms are normalized by the maximum value of the R-term for both cases.

Despite the same thermochemical properties for both cases, except for the type of the diluent used, the transport budgets of cases S-H₂O and S-N₂

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are different. Figure 2.10a shows that D and R terms have the same order of magnitude in the upstream regions of the reaction zones ($T < 1300$ K), which suggests that the flame propagation stabilization mechanism stabilizes the flame. On the other hand, for the S-N₂ case, Fig. 2.10b shows that the R term is the dominant term even in the upstream regions of the flame base, meaning that the N₂ diluted flame is stabilized mainly by the autoignition stabilization.

Even though the results of Sec. 2.4 showed that the steam dilution does not have a significant effect on the overall flame structure, the different transport budgets between the two cases suggest that the different reaction rates and species distributions of S-H₂O alters the stabilization mechanism of the flame.

2.6 Effect of steam dilution and pressure on the ignition delay time

As mentioned previously in Sec. 2.1, pressure is another important parameter for DNS studies of combustion. Even though it is known that pressure can affect flame features, DNS with high resolutions are limited with moderate pressures due to computational cost. Since it was shown in the previous section that steam dilution could alter the rate of chemical reactions, in this section, its effect on ignition characteristics of H₂-O₂ flames under different pressures is investigated using 0D gas reactor simulations.

Simulations are conducted using the constant pressure homogeneous gas reactor module of CHEMKIN-PRO, and ignition delay time (τ_{ign}) is defined as the time when the steepest temperature is observed throughout the simulation. The detailed chemical mechanism of Li et al. [71], which consists of 9 species and 21 reactions, is used for all of the analyses. Initial molar fractions of fuel, oxidizer, and diluent are based on the next-generation hydrogen gas turbine conditions, which uses pure hydrogen as fuel, and the oxidizer

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consists of 12% of O_2 and 88% of H_2O by mole. To investigate the effect of steam dilution on the ignition characteristics, analyses are also conducted for N_2 dilution, a conventional diluent that is extensively studied for hydrogen/air combustion. Since one of the possible reasons that can cause steam diluted flames to behave differently is the high efficiency factor (ε) of H_2O , an artificial diluent, H_2O_{mod} , is created by changing the ε of steam for all of the third-body and fall-off reactions in the chemical mechanism to be the same as N_2 to evaluate the sole effect of third-body efficiency factor.

In Sec. 2.6.1, simulations are conducted for all three diluents over a wide range of mixture fractions at constant pressures 1, 5, 10, and 50 atm. The initial temperatures of the fuel (H_2) and the oxidizer (O_2 and diluent) are chosen to be 300 K and 1100 K, respectively, and the initial temperature is defined by the cold mixing temperature of the mixture at every ξ . Finally, in Sec. 2.6.2, analyses are conducted for mixtures at stoichiometry and for a wide range of pressure values for a constant initial temperature of 900 K to investigate the effect of the steam on the behavior of τ_{ign} with respect to pressure.

2.6.1 Ignition characteristics over the mixture fraction domain

Figure 2.11 shows τ_{ign} as a function of mixture fraction, ξ , for three diluents. The cold mixing temperatures of the mixtures at each ξ value are also plotted with a gray line on the figures. The mixture fraction that has the lowest ignition delay time for a constant pressure is called the most reactive mixture fraction (ξ_{MR}), and the corresponding ignition delay time is called as τ_{ref} . These values are denoted with a star-shaped marker in Fig. 2.11. This figure shows the differences in the general trend of plots in the mixture fraction space for different diluents and reveals the effect of steam dilution on the ignition characteristics. As can be seen from Fig. 2.11a, the steam diluted case shows a decrease in τ_{ign} with increasing pressure, and the plots show

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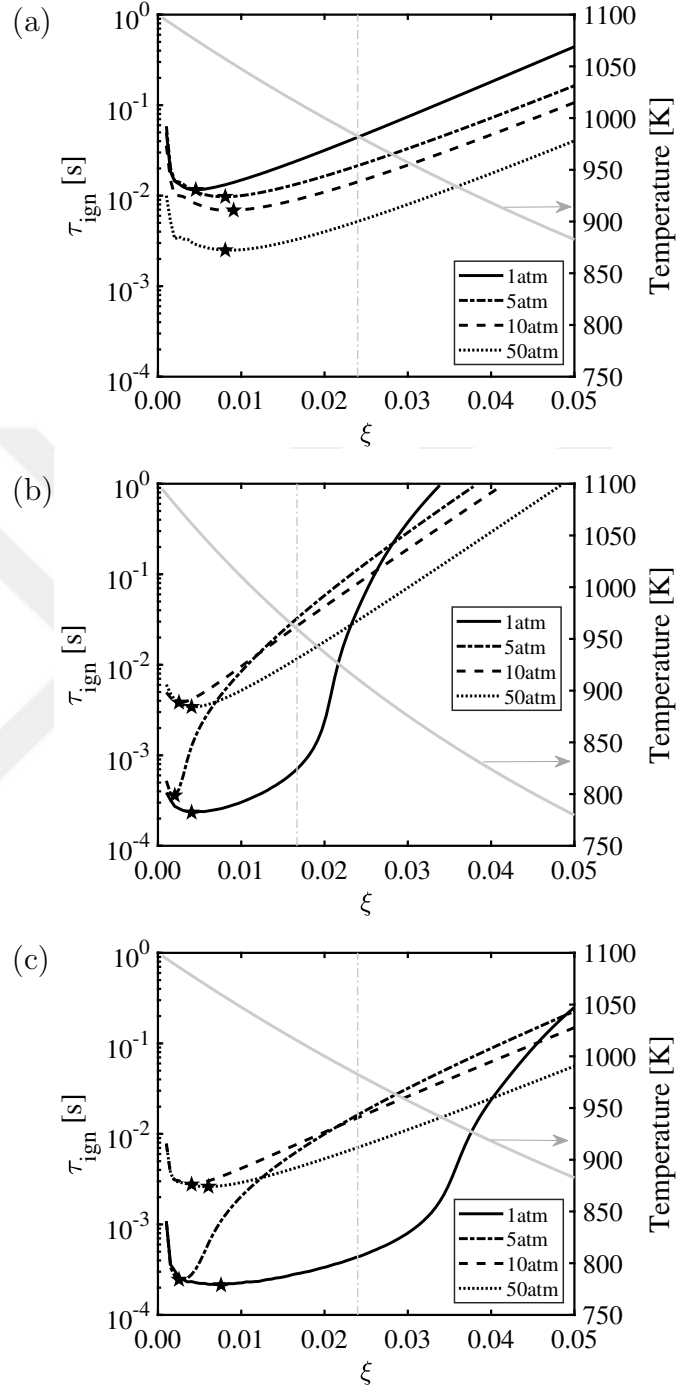


Figure 2.11: Ignition delay times of the homogeneous mixtures of H₂, O₂ and (a) H₂O, (b) N₂, and (c) H₂O_{mod} at different pressures. Temperature plot is the cold mixing temperature (Vertical line: ξ_{st} , $\star$: ξ_{MR})

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a steep decrease in τ_{ign} with increasing ξ before ξ_{MR} and a gradual increase after that for all pressures. On the other hand, it can be seen from Fig. 2.11b and 2.11c that the trend of the plots for other diluents are different from the steam diluted case, especially for pressures 1 and 5 atm. After the ξ_{MR} point, plots for 5 atm pressure show a steep increase followed by a gradual increase in τ_{ign} , and 10 atm plots show a gradual increase followed by a steep one in τ_{ign} for diluents N_2 and H_2O_{mod} .

The similarity of the general trend in the ignition delay curves and τ_{ref} of both H_2O_{mod} and N_2 diluted cases, which are significantly different from the steam diluted case, suggests that the high efficiency factor of H_2O in third-body and fall-off reactions affect the chemistry significantly. The quantitative difference between H_2O_{mod} and N_2 as seen in Fig. 2.11b and 2.11c is due to the higher heat capacity of steam, compared with N_2 , which results in higher initial mixing temperatures, causing H_2O_{mod} to be more ignitable even at higher mixture fractions.

The temporal evolution of the molar fractions of certain intermediate species at the most reactive mixture fraction for all diluents at 1 atm is plotted in Fig. 2.12, to understand the difference in τ_{ref} for steam and other diluents at lower pressures. Judging from the molar fraction evolution plots, N_2 and H_2O_{mod} dilution have similar trends, whereas the H_2O dilution follows a different trend, especially before ignition. Elementary reaction analyses show that the fastest reactions before ignition (listed in Table 2.4) for all cases are the chain reactions; R3, R1, and R2 in order. However, there is also another reaction, R9, that is as fast as these three chain reactions, and this fall-off reaction is the one that causes the main difference between the steam diluted case and the other cases. R9 is the fourth fastest reaction for N_2 and H_2O_{mod} diluted cases, following the chain reactions. However, the high efficiency factor of H_2O enables this reaction to compete with the fastest reaction R3 for the steam diluted case. As can be seen from Fig. 2.12a, this results in the accumulation of HO_2 before ignition and lower levels of H.

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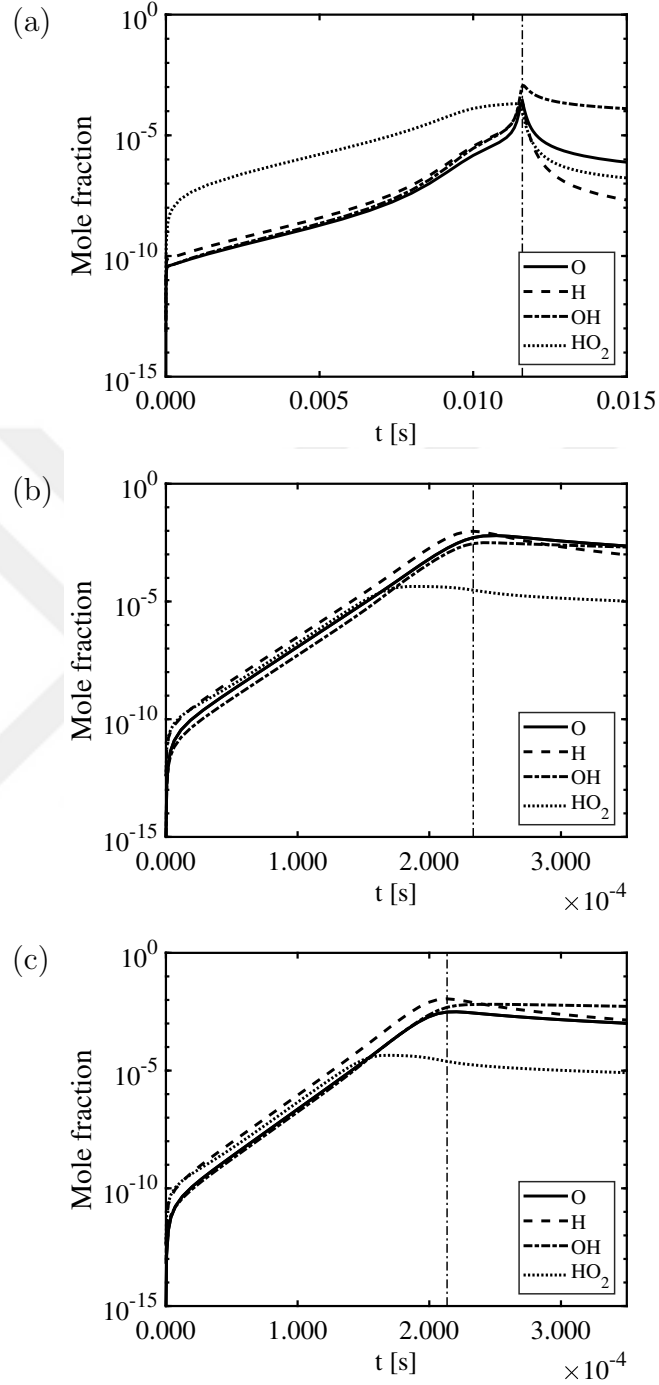


Figure 2.12: Molar fraction evolution of certain intermediate species for mixtures diluted with (a) H_2O , (b) N_2 , and (c) H_2O_{mod} at $\xi = \xi_{MR}$ and $P=1$ atm. Vertical line represents τ_{ign} .

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Table 2.4: Chemical reactions mentioned for chemical pathway analyses.

R1	$\text{H} + \text{O}_2 = \text{O} + \text{OH}$
R2	$\text{O} + \text{H}_2 = \text{H} + \text{OH}$
R3	$\text{H}_2 + \text{OH} = \text{H}_2\text{O} + \text{H}$
R4	$\text{O} + \text{H}_2\text{O} = 2\text{OH}$
R9	$\text{H} + \text{O}_2 (+\text{M}) = \text{HO}_2 (+\text{M})$
R11	$\text{HO}_2 + \text{H} = 2\text{OH}$
R15	$\text{H}_2\text{O}_2 (+\text{M}) = 2\text{OH} (+\text{M})$

The reason for these differences is that for H₂O diluted case, R9 becomes the primary H consumption reaction for the steam diluted case, whereas, for the N₂ and H₂O_{mod} diluted cases, R9 is not a significant reaction for H consumption. Consumption of H through R9 also decreases other radicals, O and OH, and therefore it works as a radical sink reaction.

Apart from the effect of high efficiency coefficient, another possible cause of the different behavior of steam diluted case, compared with other diluents, is the involvement of H₂O in the chemical reactions. Reaction analyses show that the biggest effect on H₂O is on R4. For H₂O and H₂O_{mod} diluted cases, R4 acts as the third-fastest reaction that produces OH due to high H₂O concentration, whereas for N₂ diluted case, its effect is negligible on OH production. However, Fig. 2.12b and 2.12c show that the amount of OH is comparable for N₂ and H₂O_{mod} diluted cases, and therefore the net contribution of R4 is negligible.

2.6.2 Effect of pressure on ignition characteristics

Although dilution dependence of ignition delay time was extensively assessed at 1 atm in the previous section, diluents also show different behaviors with increasing pressure values. It was previously shown that ignition characteristics changes between high and low pressures when hydrogen is burned with air [82], and Santner et al. [83] studied the effect of water vapor addition on the burning rates of H₂ mixtures at pressures between 1-10 atm. How-

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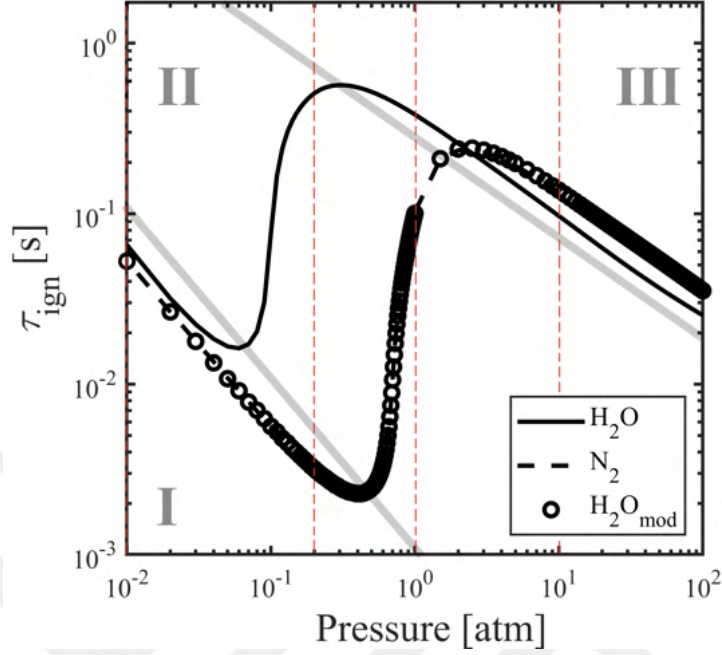


Figure 2.13: Change of ignition delay times of mixtures with different diluents with respect to pressure. Vertical lines correspond to the pressures investigated in Fig. 2.14 to evaluate the molar fractions. Thick gray lines roughly separate the τ_{ign} -pressure regimes.

ever, the effect of water vapor on the ignition delay times of hydrogen-oxygen combustion over a wide pressure range is still unknown. In this section, ignition delay times of steam diluted hydrogen-oxygen mixture is compared with other diluents over a wide range of pressure.

Figure 2.13 shows ignition delay times with respect to pressure, and ignition delay times for all three diluents exhibit an S-shaped behavior as pressure changes. The S-shaped plot distinguishes three regimes with high- and low-pressure limits. These regimes are roughly separated from each other with thick gray lines in Fig. 2.13, and named with roman numerals. The first regime (I) corresponds to low pressures, where ignition delay time decreases with pressure. After the low-pressure limit is hit, the second regime (II) starts with a steep increase in ignition delay time until the high-pressure limit. Finally, after the high-pressure limit, the third regime (III) starts, and

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the ignition delay time decreases again with increasing pressure. Comparing the behavior of three diluents show that H_2O enters the second pressure regime at lower pressures than the other two diluents, and the fact that N_2 and H_2O_{mod} diluted cases follow almost exactly the same plot line suggests that the high third body efficiency factor of steam is responsible for this difference, rather than its high heat capacity or other possible factors.

To further investigate the differences between three diluents, the mole fraction of each diluent case's intermediate species and temperature evolution at different pressures are plotted in Fig. 2.14. Pressures shown in Fig. 2.14 are selected so that there will be at least one case for all three pressure regimes of all diluents, and corresponding pressures are shown with vertical lines in Fig. 2.13. Figures 2.14a, 2.14b, and 2.14c show the results for the 0.01 atm case, which corresponds to the first regime for all diluents. At this pressure, ignition delay times of all cases are almost the same, as can be seen from Fig. 2.13. Figures 2.14a, 2.14b, and 2.14c show that the mole fractions of the species are almost the same before ignition. The most significant difference is observed in the amount of HO_2 . Steam diluted case have higher HO_2 levels as the primary production reaction for HO_2 is the fall-off reaction, R9, and its rate is higher because of steam's high efficiency factor. However, the effect of high ε in this region is not as significant as the case mentioned in the previous section. Even though the rate of R9 has increased, chemical reaction analyses show that it is still the fourth fastest reaction for every case.

Figures 2.14d, 2.14e, and 2.14f show the plots for the pressure at 0.2 atm. At this pressure, the steam diluted case falls into the second pressure regime, whereas N_2 and H_2O_{mod} diluted cases are still on the first regime. A steep increase in the ignition delay time in this region causes the steam diluted case to have a higher ignition delay time than other diluents. A clear difference between Figs. 2.14d and 2.14e is also present. The most distinctive difference is observed for the HO_2 radical. HO_2 has a significantly higher mole fraction

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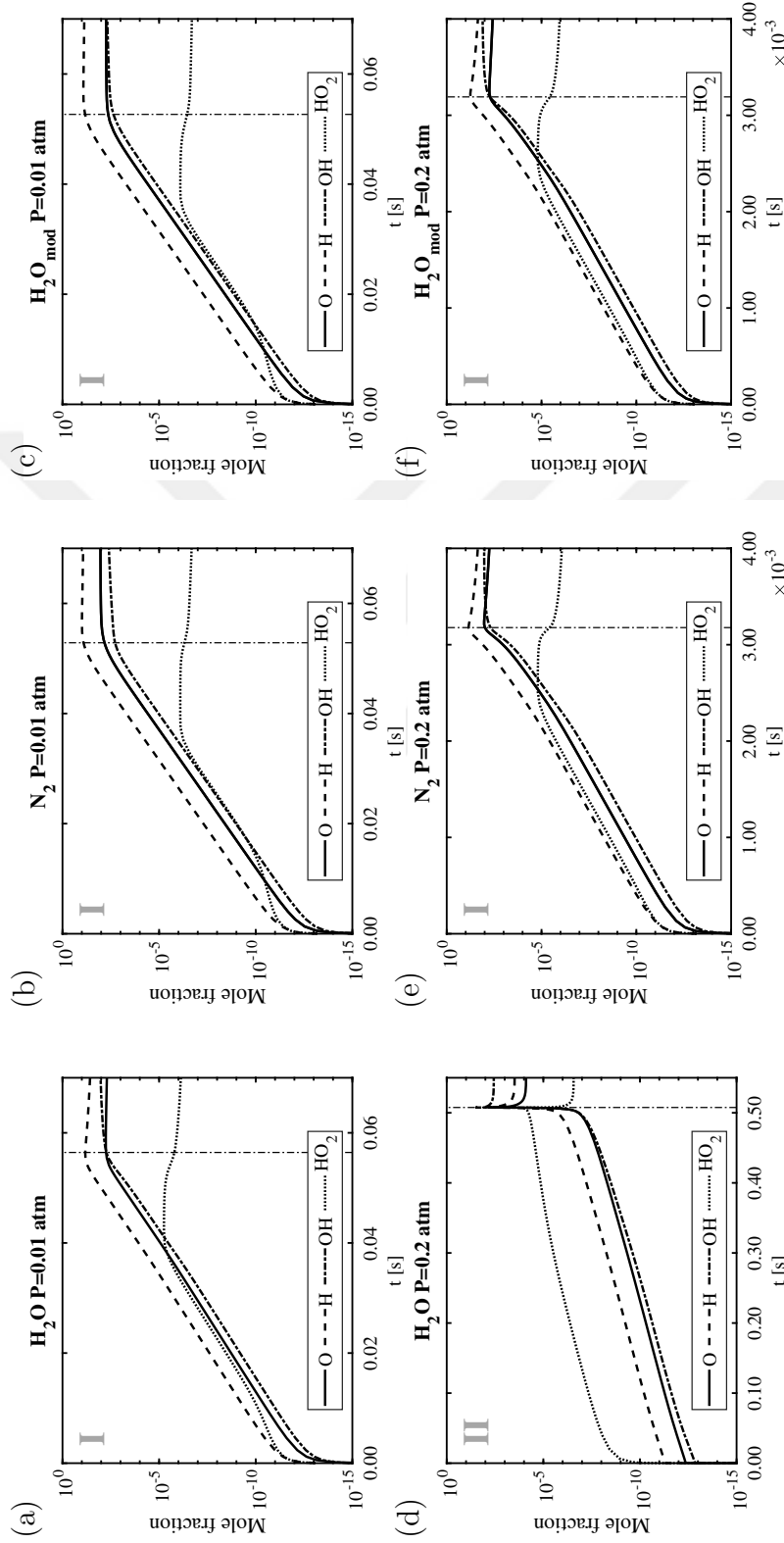


Figure 2.14: Evolution of molar fraction of intermediate species for (a,d) H_2O diluted, (b,e) N_2 diluted, and H_2O_{mod} diluted (c,f) mixtures at (a,b,c) 0.01 atm, (d,e,f) 0.2 atm. Vertical lines denote τ_{ign} . The roman numerals on the upper left side of each plot correspond to the regimes on the τ_{ign} against pressure plot. (continued)

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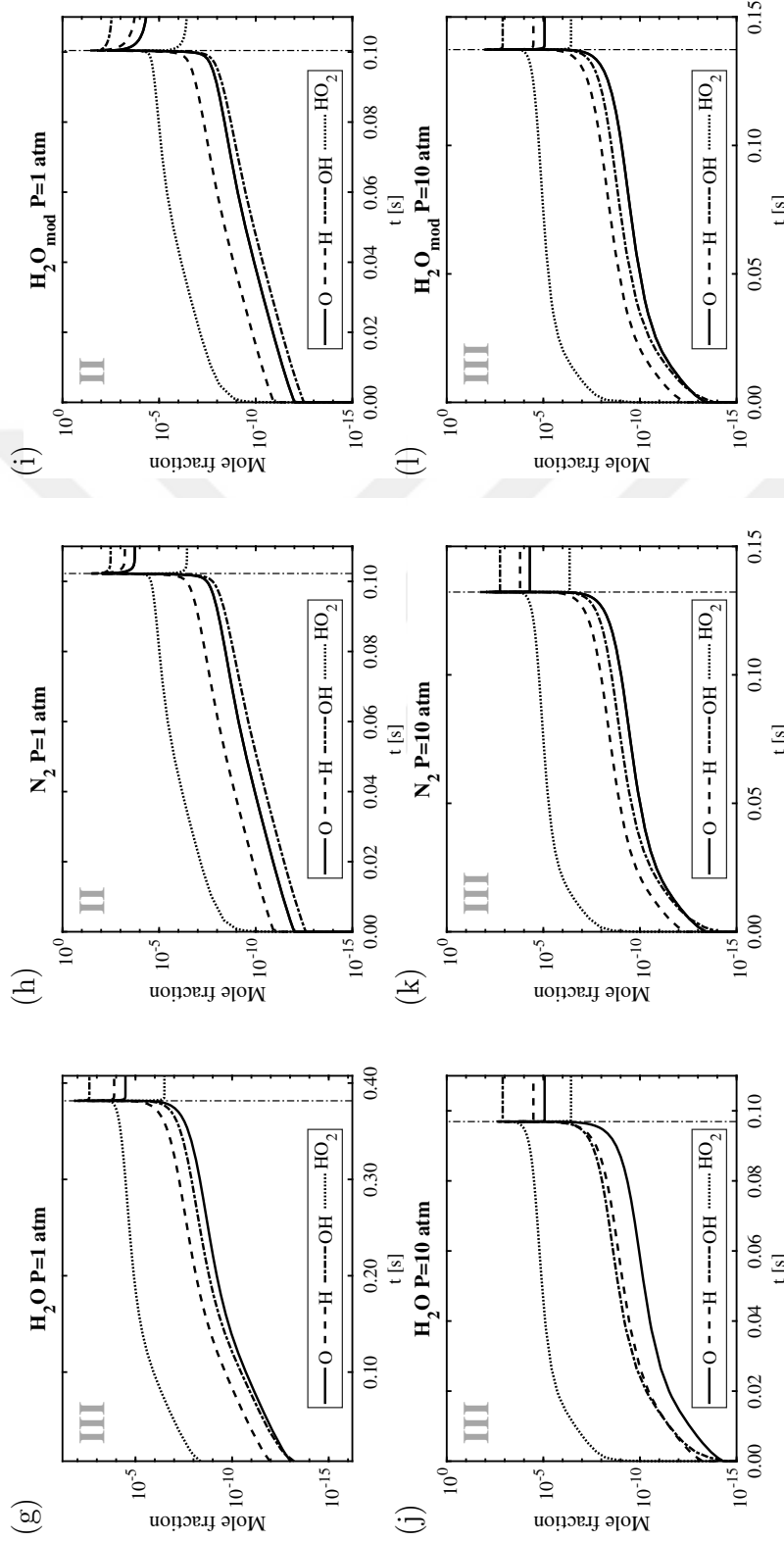


Figure 2.14: (*continued*) Evolution of molar fraction of intermediate species for (g,j) H₂O diluted, (h,k) N₂ diluted, and H₂O_{mod} diluted (i,l) mixtures at (g,h,i) 1 atm, (j,k,l) 10 atm. Vertical lines denote τ_{ign} . The roman numerals on the upper left side of each plot correspond to the regimes on the τ_{ign} against pressure plot.

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than other radicals for the steam diluted case, whereas, for other diluents, HO_2 does not even have the highest mole fraction value. Elementary reaction analyses show that R9 at 1 atm becomes so fast for the steam diluted case that the main HO_2 consumption reaction, R11, cannot compete with it even though its rate increases with time. Whereas, for other diluents, the rate of R11 is closer to R9 and its increasing rate even catches R9 after about 0.1 ms, causing HO_2 mole fraction to become almost constant. This trend is also observed for all diluents at 0.01 atm when they are all still on the first pressure regime. The increased rate of R9 in the second regime for the steam diluted case also makes it the main consumption reaction for H radical, decreasing the amount of H before ignition.

At the atmospheric pressure, as shown in Figs. 2.14g, 2.14h, and 2.14i, steam is in the third, and other diluents are in the second regime. The most significant difference between 1 atm and 0.2 atm pressures, especially for N_2 and H_2O_{mod} diluted cases, is the amount of HO_2 mole fraction. In this region, R9 becomes competent with the fastest reaction, R3, even for these diluents, making HO_2 the radical that has the highest mole fraction value in the pre-ignition zone, just like the steam diluted case at 0.2 atm. However, the high ε value of steam makes R9 faster than other diluents, resulting in relatively higher HO_2 accumulation. A high rate of R9 results in similar outcomes as before, decreasing the amount of H and consecutively O radical. Another essential difference is observed for the steam diluted case. At 1 atm, which falls into the third pressure regime for steam dilution, the fall-off reaction, R15, becomes the primary reaction responsible for OH, surpassing even the chain reactions R1 and R2. This results in a significant increase in OH amount, and the OH mole fraction becomes higher than O.

At 10 atm, shown in Figs. 2.14j, 2.14k, and 2.14l, all cases with different diluents fall into the third pressure regime, where τ_{ign} decreases with pressure, and they all have similar τ_{ign} values. In this region, R15 becomes the main reaction for OH production for N_2 and H_2O_{mod} diluted cases too, but high ε

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of steam makes this reaction more important than the other OH production reactions, R1 and R2, resulting in slightly lower O and H mole fractions.

2.7 Effect of pressure on the flame structure

In Sec. 2.6, it was shown that pressure might change the ignition characteristics, which may result in a change in the structure and stabilization of the lifted flames. Therefore, in this section, laminar lifted single jet flames under nominal gas turbine thermochemical conditions and four different pressures (2-20 atm) are simulated to study the effect of pressure on the flame structure. The structure of the flames is investigated using the $\dot{Q}$ and NFI distributions, similar to Sec. 2.4.

Figure 2.15 shows the $\dot{Q}$ contours of all cases for significant $\dot{Q}$ regions. Flame thickness decreases with increasing pressure, as expected. Maximum $\dot{Q}$ values increase with the pressure, as can be seen from the limits of the legends. This is due to the increase in the rate of reactions with pressure. An increase in diffusion may also increase $\dot{Q}$, by providing more reactants to the reacting regions. The $\dot{Q}$ contours of all cases are similar to the S-H₂O and S-N₂ cases. The maximum heat release rate is observed around the flame base, slightly towards the rich regions. The high diffusivity of H_2 shifts the ξ_{st} iso-lines towards the oxidizer, resulting the diffusion and lean premixed branches to collide.

Figure 2.16 illustrates the NFI contours of all cases for significant $\dot{Q}$ regions. NFI contours reveal the typical tribrachial structure of the lifted flames. The lean premixed and diffusion flames, which could not be distinguished from one another in Fig. 2.16 is clearly seen in Fig. 2.16.

The probability density function of ξ , as well as the conditional averages of $\dot{Q}$ and the NFI are illustrated in Fig. 2.17 to elucidate the flame structures of the high pressure flames. The PDF distribution of all cases, shown in Fig. 2.17a peaks around the ξ_{st} , corresponding to the diffusion flame. This

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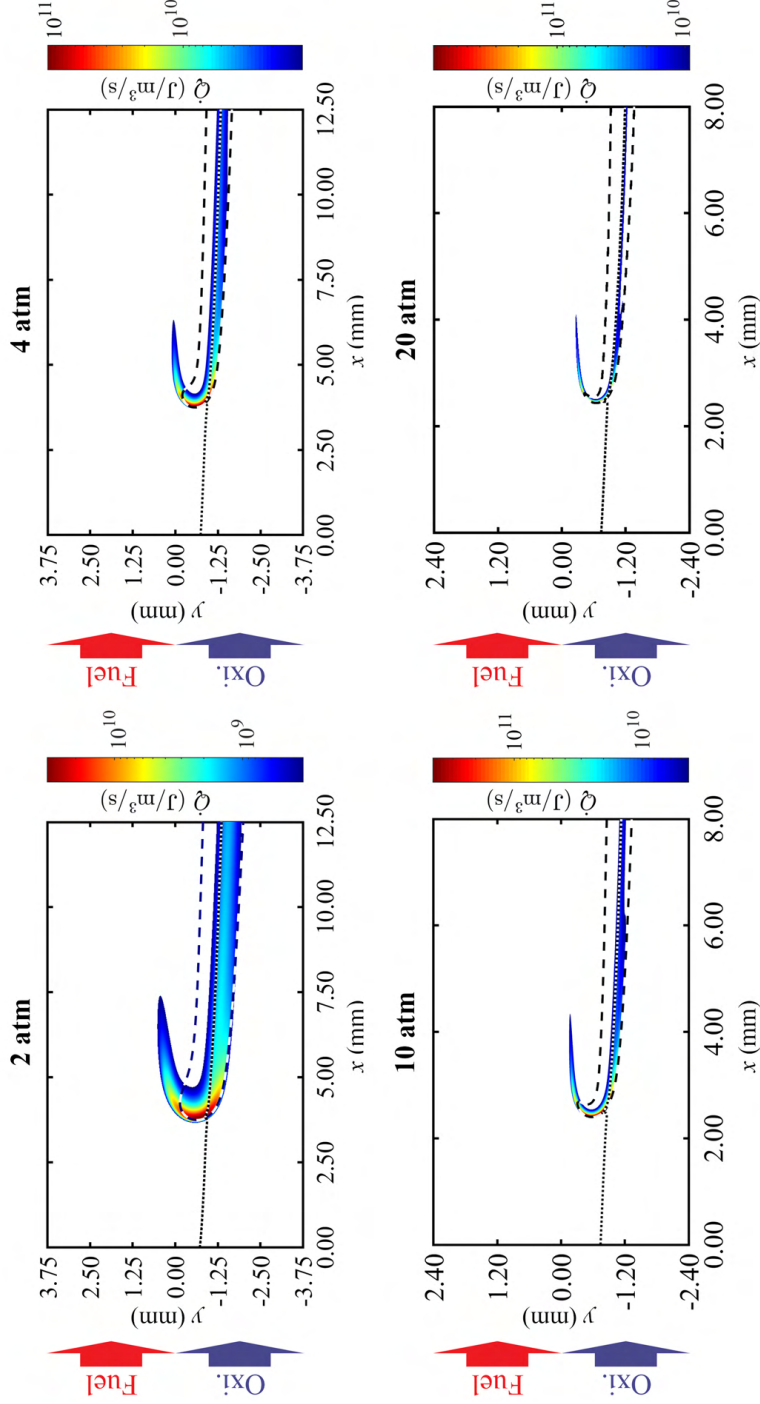


Figure 2.15: Logarithmic heat-release rate ($\dot{Q}$) contours of cases with higher pressures. Contours are shown for regions with a substantial heat-release rate, $\dot{Q} > 0.01\dot{Q}_{max}$. The dashed and dotted lines correspond to $Y_{OH} = Y_{OH,5\%}$ and ξ_{st} iso-lines, respectively.

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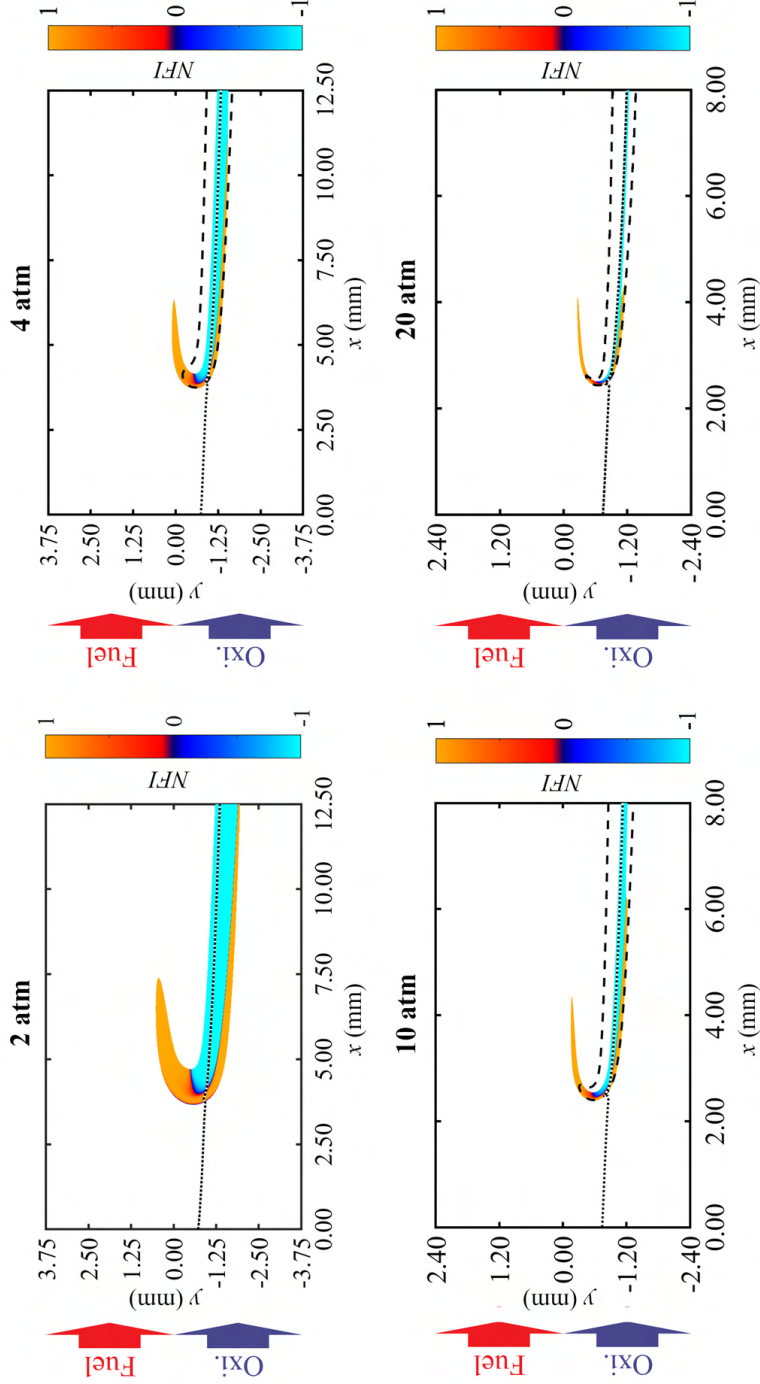


Figure 2.16: Normalized flame index (NFI) contours of cases with higher pressures. Contours are shown for regions with a substantial heat-release rate, $\dot{Q} > 0.01\dot{Q}_{max}$. The dashed and dotted lines correspond to $Y_{OH} = Y_{OH,5\%}$ and ξ_{st} iso-lines, respectively.

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peak corresponds to the diffusion flame, trailing along the ξ_{st} iso-line, which can be understood from the negative NFI values in Fig. 2.17b. As the pressure increases, the peak value in the PDF decreases, showing a slightly wider distribution towards leaner regions.

The mean NFI values conditioned on ξ (Fig. 2.17b) show positive values on lean and rich sides and negative values around ξ_{st} , revealing the tribrachial flame structure. The mean values of $\dot{Q}$, conditioned on ξ , show two peaks for all cases. The first peak is observed for lean regions. The second and the highest peak is observed for rich premixed flames. The mean $\dot{Q}$ values increase with pressure, as previously observed in Fig. 2.15. Both the NFI and $\dot{Q}$ plots show a wider distribution along the ξ domain with increasing pressure. This is a result of thinner reaction zones, resulting in larger scalar gradients.

The visual inspections and statistical analyses of the laminar lifted single jet flames for different pressures show that pressure has a slight qualitative effect on the flame structure. The flame thickness decreases, resulting in larger scalar gradients inside the reaction zones. The $\dot{Q}$ is also increased by pressure. However, the overall flame structure remains the same. All cases show a tribrachial flame structure with collapsed lean premixed and diffusion flames.

2.8 Effect of pressure on the flame stabilization

The results of Sec. 2.7 showed that pressure does not have a significant effect on the flame structure. However, pressure increases the $\dot{Q}$ values in the reaction zones, which may, in turn, change the stabilization mechanism. To investigate the effect of pressure on the flame stabilization mechanism, the transport budget of Y_{OH} along the ξ_{st} iso-line is calculated for every pressure case, and the results are illustrated in Fig. 2.18.

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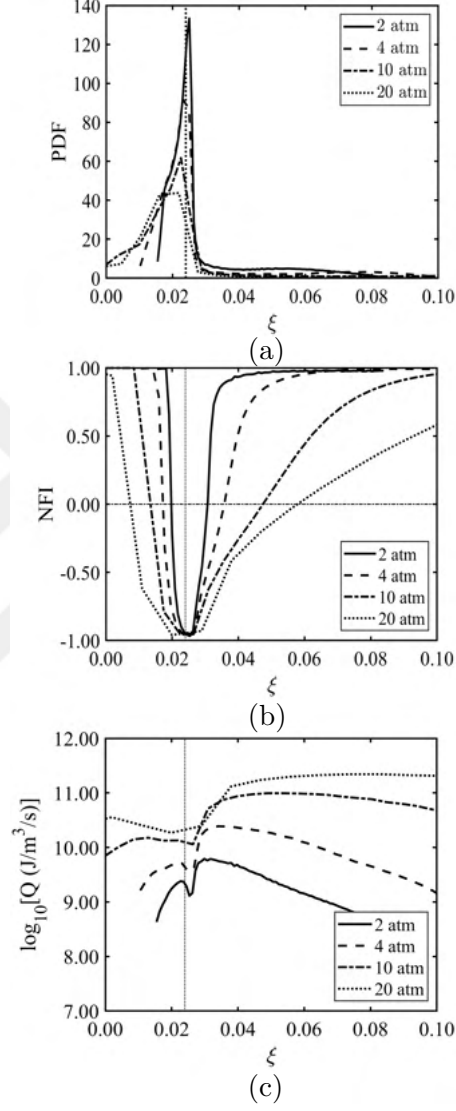


Figure 2.17: PDF of mixture fraction (ξ) (a), and average values of the normalized flame index (NFI) (b) and heat-release rate ($\dot{Q}$) (c) conditioned on ξ for higher pressure cases. The vertical lines correspond to ξ_{st} . Only samples that have substantial $\dot{Q}$ values ($\dot{Q} > 0.01\dot{Q}_{max}$) are used.

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The transport budget for the 2 atm case shows a similar trend with the S-H₂O case, which suggests that the flame at 2 atm is stabilized by the flame propagation stabilization mechanism. The magnitude of the diffusion term increases as the pressure increases. The most significant increase is observed for the upstream of the reaction zones, which characterizes the preheat zone. This kind of behavior is typical to the propagating flames and shows that the flame propagation stabilization mechanism stabilizes the flames under nominal gas turbine conditions, even at high pressures.

The increase of D-term in both directions means that more species are transported to the upstream and downstream of the reaction zones, which increases the reaction rates as well. This behavior is clearly seen in Fig. 2.18, as R-term increases with D-term. This increase in reaction rates also explains the high $\dot{Q}$ observed for higher pressures, as observed in Figs. 2.15 and 2.17c.

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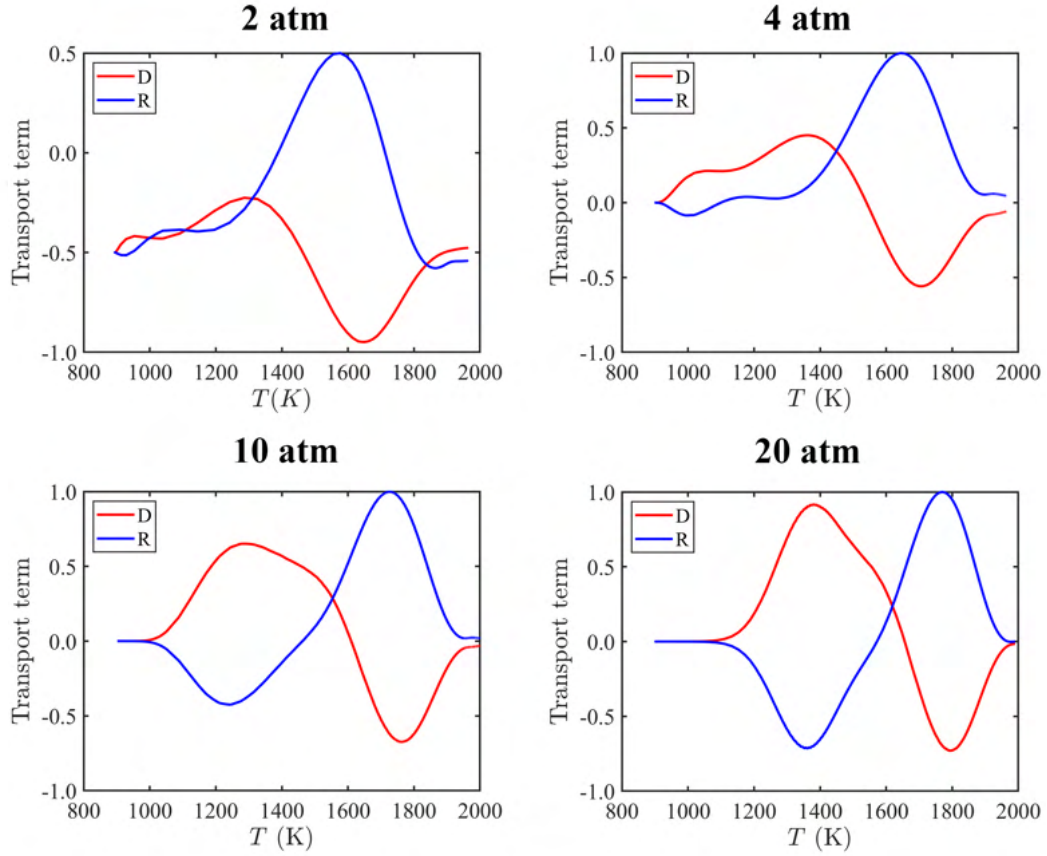


Figure 2.18: Transport budget of Y_{OH} along the ξ_{st} for every pressure case. The transport terms are normalized by the maximum value of the R-term for each case.

2.9 Interim conclusions

Effect of steam dilution and pressure on the fundamental features of lifted flames of H₂ and O₂ is investigated using canonical laminar DNSs and a homogeneous gas reactor model.

Initially, an H₂O diluted case is compared with an N₂ diluted case using DNS. The $\dot{Q}$, NFI , and T fields and their statistical analyses showed that both cases show similar structures overall. Furthermore, the tribrachial structure, which is typical of lifted flames, is observed in both cases, whereas the high diffusivity of H₂ caused the collapse of the diffusion and the lean premixed flames. However, even though the overall flame structures of both cases are similar, the reaction rate analyses show differences between the two cases. The high efficiency factor of H₂O and the involvement of steam in the chemical reactions increased the rate of certain reactions.

The transport budget analyses reveal that the flame propagation stabilization mechanism is stabilizing the H₂O diluted case, while autoignition is the dominant stabilization mechanism for the N₂ diluted case. This difference is a possible result of the steam dilution, which alters the rate of certain reactions.

The homogeneous gas reactor analyses conducted to investigate the effect of steam dilution on ignition characteristics under different pressures. The results showed that even though the high heat capacity and low molecular weight of H₂O, compared with N₂, is affecting the ignition delay times, the most significant difference is caused by the high efficiency factor of steam, which is 11-12 times higher than N₂. These analyses also show that the involvement of H₂O in the chemical reactions does not significantly affect the ignition delay times of the mixtures. The change in the ignition delay time with pressure is investigated using similar analyses. The results reveal that the ignition delay time shows a non-monotonic behavior with increasing pressure, which may result in a change in the stabilization mechanism of lifted

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flames under higher pressures. The high efficiency factor of steam shifts this non-monotonic curve towards the lower pressures.

The effect of pressure on the flame features of lifted flames under nominal gas turbine thermochemical conditions is investigated for four different pressures (2-20 atm) using DNS. The structure and stabilization mechanisms of flames under different pressures show similarities, suggesting that the pressure does not affect the fundamental flame features of lifted flames under current thermochemical conditions.



Chapter 3

Laminar multi-jet flames of H_2 and O_2 diluted with steam

3.1 Preface

In many practical gas turbines, the fuel and oxidize enters the combustion chamber from multiple jet exits to enhance mixing, potentially producing multiple lifted-flame bases. Consequently, these flames might interact with one another, resulting in complex flame structures. To investigate the effect of such possible interactions on the flame features, without the influence of turbulence, DNSs of two-dimensional laminar flames under nominal gas turbine thermochemical conditions are performed in this chapter. Two cases with different domain sizes are investigated to observe the effect of jet separation.

In Sec. 3.2, the domains constructed for both cases are explained. In Sec. 3.3, the flame structures are investigated using the $\dot{Q}$ and NFI fields and their statistical analyses over ξ domain. In Sec. 3.4, the stabilization mechanisms of both cases are investigated in comparison to the single-jet flame of the same conditions, presented in Ch. 2. The transport budget of Y_{OH} along the ξ_{st} iso-line is used to determine the flame stabilization mechanism. Finally, the conclusions of this chapter are listed in Sec. 3.5.

3.2 Domain configurations

The domains are configured to have periodic boundaries in transverse directions, and the fuel is issued from the inlet in the form of half jets centered at the transverse boundaries. Therefore, these half jets are expected to undergo an interaction that depends on their separation, providing basic information about the structure of multi-jet flames.

Two values for the jet-center separation are considered and referred to as Case I and Case II. The fuel is pure H_2 at 288 K, and the oxidizer consists of 12% O_2 and 88% H_2O by mole at 916.5 K. The thermochemical conditions, except for the pressure, correspond to those of a next-generation hydrogen gas-turbine engine, having a thermal efficiency of 75% [74]. The pressure is set to 2 atm, and the initial inflow velocity is set to 10 m/s at $x = 0$ for both Case I and Case II. The inflow velocity is adjusted to maintain the flame base at a certain position. After the solution reaches a steady-state, the final inflow velocity is 7.91 m/s and 7.80 m/s for Case I and Case II, respectively.

The domain size is $L_x \times L_y = 14.00 \times 7.00 \text{ mm}^2$ and $14.00 \times 4.95 \text{ mm}^2$ for Case I and Case II, respectively. L_y corresponds to the jet separation because the jet centers are positioned at the periodic boundaries. Both domains are discretized by $N_x \times N_y = 1156 \times 640$ uniform mesh points. The inflow boundary at $x = 0$ and the outflow boundary at $x = L_x$ are specified using Navier–Stokes characteristic boundary conditions (NSCBC) [73]. The transverse boundaries are described above.

The scalar profiles at the inlet are specified by the following tangential profile, which is similar to that considered in Ref. [47]:

$$q_{in} = q_c + \frac{q_j - q_c}{2} \left[\tanh \left(\frac{y - L_y + H/2}{2\delta} \right) - \tanh \left(\frac{y - H/2}{2\delta} \right) \right], \quad (3.1)$$

where the generic quantity q corresponds to the scalars, such as temperature and mass fractions of H_2 , O_2 , and H_2O . The subscripts j and c correspond to the fuel jet and oxidizer co-flow, respectively. Here, H denotes the jet width,

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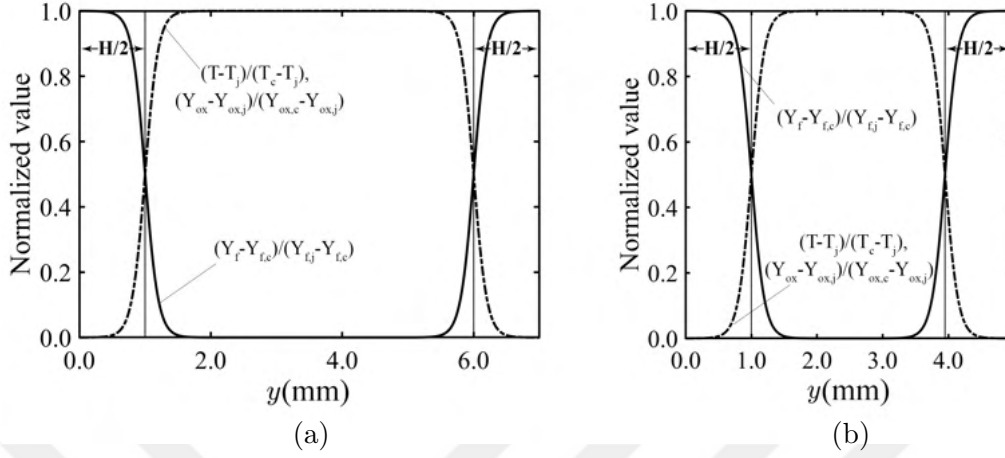


Figure 3.1: The inflow profiles for (a) Case I and (b) Case II.

$H = 2$ mm, and δ is set to be 5% of H . The inflow profiles for Case I and Case II are shown in Fig. 3.1.

3.3 Structure of laminar multi-jet flames

Similar to the laminar lifted single-jet flames, presented in Sec. 2.4, $\dot{Q}$ and NFI distribution is investigated to reveal the flame structure of laminar lifted multi-jet flames. Figures 3.2a and 3.2b show the logarithmic heat-release rate ($\dot{Q}$), and Figs. 3.2e and 3.2f show the normalized flame index (NFI) contours for regions with a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) of both cases.

The figures are super-imposed with iso-lines of the stoichiometric mixture fraction ($\xi_{st} = 0.025$) and OH mass fraction corresponding to 5% of its maximum value ($Y_{OH} = Y_{OH,5\%}$), and their intersection is defined as the flame base location of the flames. Additionally, in the present study, flame-base regions are defined based on areas with a high heat-release rate, $\dot{Q} > 0.3\dot{Q}_{max}$, in such a way that these regions include all flame-base positions. Fig. 3.2c and 3.2d show the flame-base positions as part of the flame-base regions of the laminar multi-jet flames.

As illustrated in Figs. 3.2a and 3.2b, the highest $\dot{Q}$ value for both Case I

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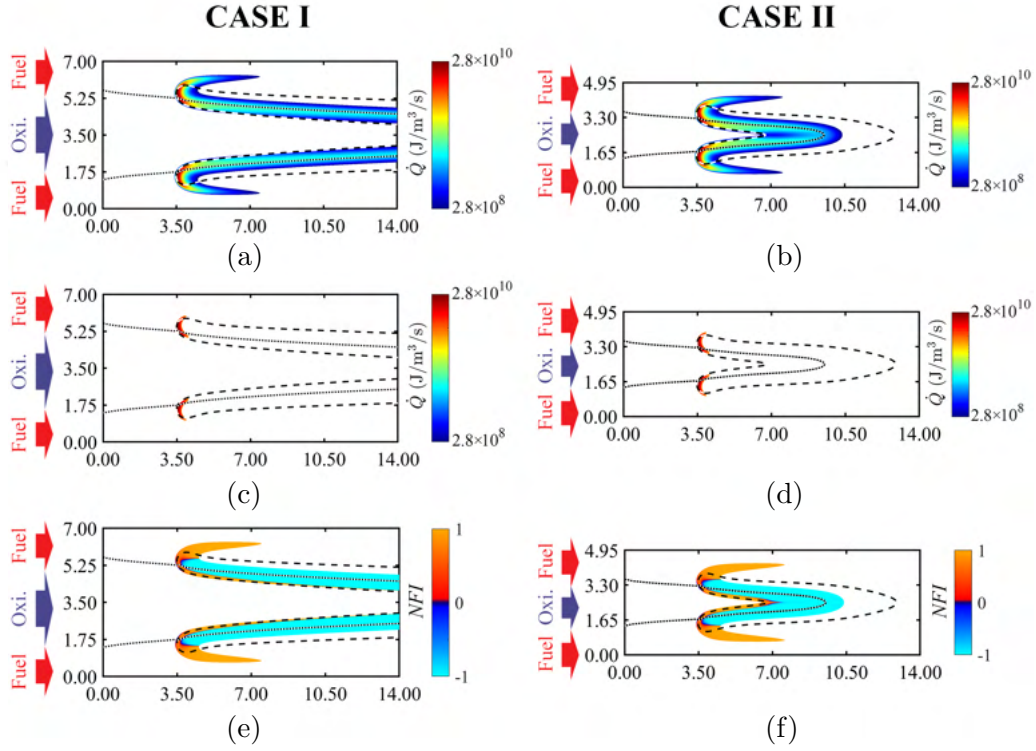


Figure 3.2: (a,b,c,d) Logarithmic heat-release rate ($\dot{Q}$), and (e,f) normalized flame index (NFI). Contours are shown for flame-base regions, with $\dot{Q} > 0.3\dot{Q}_{max}$ (c,d), and for regions with a substantial heat-release rate, $\dot{Q} > 0.01\dot{Q}_{max}$ (a,b,e,f). (a,c,e) Case I, and (b,d,f) Case II. The dashed and dotted lines correspond to $Y_{OH} = Y_{OH,5\%}$ and ξ_{st} iso-lines, respectively.

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and Case II occurs approximately at the flame-base locations, slightly on the rich side ($\xi > \xi_{st}$) of the domain. Based on the heat-release rate contours in Figs. 3.2a and 3.2b, the lean premixed and diffusion flame branches of the flames in both cases cannot be distinguished from each other. This feature is caused by the high diffusivity of H_2 , which shifts ξ_{st} towards the lean side ($\xi < \xi_{st}$). A similar behavior was observed for single flames as well, and the reasons were discussed previously in Sec. 2.4.

Figure 3.2e and 3.2f show the NFI contours at the regions with a substantial heat-release rate for Case I and Case II, respectively. Figure 3.2e reveals that Case I has the typical tribrachial structure of the non-premixed lifted flames. The premixed flame branches are observed on the lean and rich sides, and the diffusion flame trails along the ξ_{st} iso-lines. Figure 3.2f depicts the NFI contours for Case II, and three flame branches are again observed. As can be expected from the $\dot{Q}$ field (Figs. 3.2a and 3.2b), the lean premixed and diffusion flame branches that conventionally trail along the ξ_{st} iso-lines downstream, merge with one another, following the merged ξ_{st} iso-lines.

Conditional averages of $\dot{Q}$ and the NFI on ξ , as well as the probability density function (PDF) of ξ , for the regions with a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) are illustrated in Fig. 3.3 for both laminar cases. This figure shows that the flame structures for Case I and Case II are similar statistically, except for a slight difference in lean regions. For both cases, there is a peak in the PDF at $\xi \approx \xi_{st}$, which corresponds to the diffusion flame branch, as can be seen by the negative NFI values in Fig. 3.3b. Moreover, for both cases, there are no peaks on the lean or rich side, reflecting the relatively small volume of lean and rich flame branches. The positive NFI values on the lean and rich sides for both cases suggest the existence of lean premixed and rich premixed flame branches, revealing the typical tribrachial flame structure of a non-premixed lifted flame together with a diffusion flame branch. The PDF values on the lean side of Fig. 3.3a are slightly lower for Case II than for Case I because the two lean premixed flame branches for

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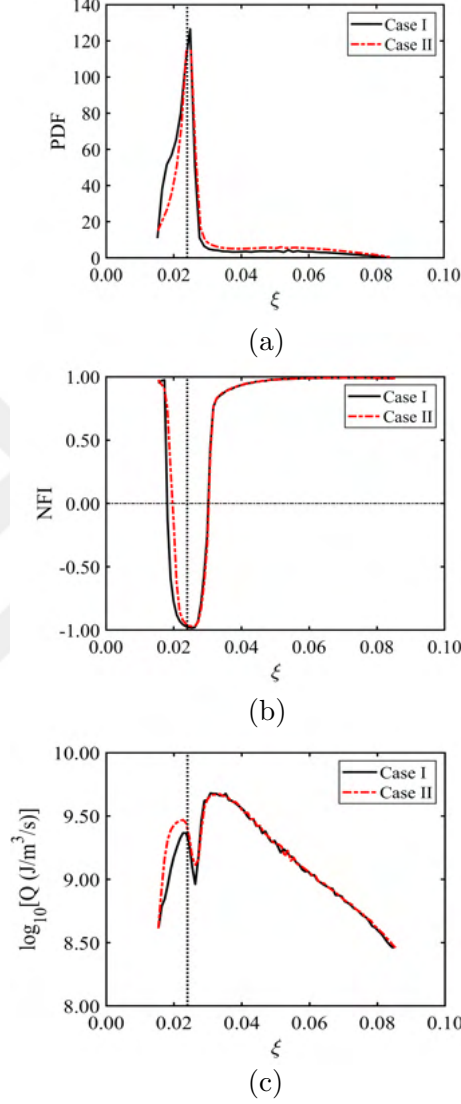


Figure 3.3: PDF of mixture fraction (ξ) (a), and average values of the normalized flame index (NFI) (b) and heat-release rate ($\dot{Q}$) (c) conditioned on ξ for the laminar cases. The vertical lines correspond to ξ_{st} . Only samples that have substantial $\dot{Q}$ values ($\dot{Q} > 0.01\dot{Q}_{max}$) are used.

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Case II merge with each other.

The mean values of the heat-release rate conditioned on the mixture fraction in Fig. 3.3c have a first peak at $\xi \approx \xi_{st}$ and a second peak at $\xi \approx 0.03$ (on the rich side) for both cases. The first peak has slightly higher $\dot{Q}$ values for Case II than for Case I, and the high $\dot{Q}$ values are observed for a wider range of ξ values. For both cases, the first peak corresponds to both the lean premixed and diffusion flame branches, as can be seen from the NFI values in Fig. 3.3b. The merged heat-release rate of these branches is a result of the high diffusivity of H_2 , which shifts the diffusion flame towards the lean premixed flame and makes the two branches collide with each other, as already discussed.

The different behaviors of the NFI , with clearly separated lean premixed and diffusion flame branches in Fig. 3.3b, and the heat-release rate, with merged branches in Fig. 3.3c, are caused by the different mechanisms of transportation, previously discussed in Sec. 2.4. For both cases, the second (and highest) peak in the conditionally averaged $\dot{Q}$ (Fig. 3.3c) corresponds to the point at which the NFI in Fig. 3.3b changes from negative to positive values. This observation suggests the existence of both premixed and diffusion flames with high heat-release rates. Finally, Figure 3.3c shows high $\dot{Q}$ values over a broad range of ξ values greater than ξ_{st} , which demonstrates that the rich premixed flame branch has a higher $\dot{Q}$ than the lean premixed flame branch on average.

3.4 Stabilization of laminar multi-jet flames

Similar to the analyses shown in Ch. 2, the transport budget of OH is analyzed along the stoichiometric mixture fraction lines of Case I and Case II, and results are illustrated in Figs. 3.4a and 3.4b respectively. Case I and Case II follow a similar trend until ≈ 1900 K, showing that jet separation distance does not affect the stabilization mechanism of the flames. Case II

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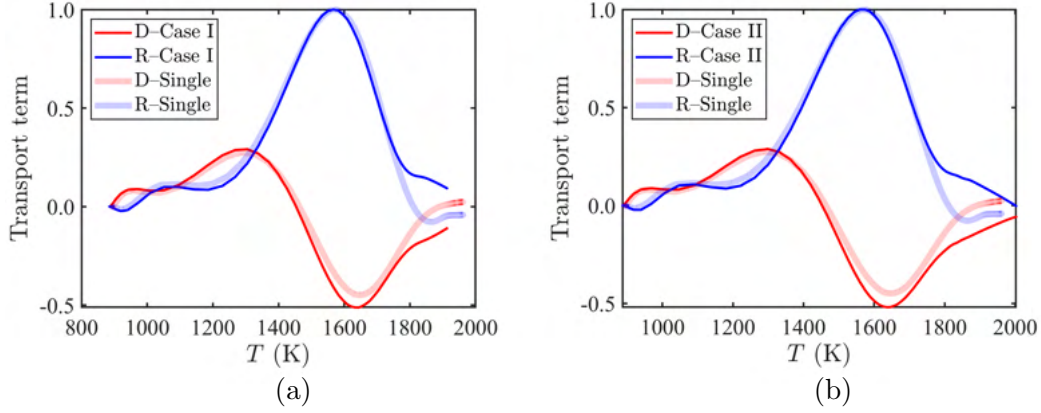


Figure 3.4: Transport budget analyses of OH along the mixture fraction line of (a) Case I and (b) Case II. The plots are super-imposed by thick transparent lines, corresponding to the OH transport budget of the single lifted flame at 2 atm, previously shown in Fig. 2.18. Transport terms are normalized by the maximum value of the R term for each case.

has higher temperatures along the ξ_{st} iso-line, which allows D-R terms to be observed for $T > 1900$ K.

The effect of multi-jets on the flame stabilization mechanism is investigated by comparing Case I and Case II with the laminar single lifted flame at 2 atm, reported in Sec. 2.8. OH transport budget of the mentioned flame, previously given in Fig. 2.18, is superimposed on Figs. 3.4a and 3.4b. The trends of both the multi-jet and single-jet cases are similar overall, with a slight difference in the downstream of the reaction zones ($T > 1600$ K). In these regions, The magnitude of the D terms of the multi-jet cases shows a slight increase, possibly caused by the interaction of neighboring jets. This increase in the D term also increases the R term. Consequently, the dominant D-R terms, which is a staple of propagation stabilized flames, is observed for downstream regions as well. Since this difference is only observed for the downstream regions, and the D-R terms are still dominant, it can be said that the laminar multi-jet flames are also stabilized by the flame propagation mechanism.

3.5 Interim conclusions

The effect of multi-jet configuration on the flame structure and stabilization mechanism is investigated using two cases with different jet separations. The visual inspections of the $\dot{Q}$ and NFI fields showed that the diffusion and lean premixed flames of the case with shorter jet separation distance merge with each other inside the domain limits, downstream the flame base regions. However, both the visual inspections and statistical analyses show that the flame structure of both cases is similar to each other, as well as the single-jet flame at 2 atm, presented in Sec. 2.7. This similarity suggests that the interaction of the flames does not have a significant effect on the flame structure under current, nominal gas turbine conditions.

The stabilization mechanism of the flames is investigated using the transport budget analysis of OH. Both cases showed similarities, suggesting that the jet separation distance does not affect the OH transport budget, thus the stabilization mechanism. Transport budgets of multi-jet cases are also compared with the single-jet flame stabilization, previously presented in Sec. 2.8. The plots showed similar trends, except for a slight difference in the downstream regions. In the downstream of the flame base, the magnitude of the diffusion term for the multi-jet cases is slightly higher than the single-jet flame under the same conditions, resulting from the flame interactions. This increase in the diffusion of the OH species accelerates the reaction, resulting in a slight increase in the reaction term, balancing the diffusion term. However, this difference is only slight and does not affect the dominant D-R balance. Thus, the transport budget analyses show that flame propagation is the dominant stabilization mechanism for the laminar multi-jet cases as well.

Chapter 4

Turbulent multi-jet flames of H_2 and O_2 diluted with steam

4.1 Preface

In Ch. 4, the multi-jet flame features are investigated without the effect of influence. However, practical combustion devices operate under turbulent conditions, which result in complex flame structures, possibly altering the flame stabilization mechanisms. Therefore, in this chapter, 3D turbulent multi-jet flames of H_2 and O_2 diluted with H_2O are investigated. The conditions are based on the nominal gas-turbine, same as Ch. 3.

In Sec. 4.2, the domain configuration of the case is summarized. Next, the flame structure and stabilization mechanism are investigated in Secs. 4.3 and 4.4 respectively. Since the turbulence results in a more complex flame base structure, flame features are investigated using a more intricate approach than the laminar flames presented in Chs. 2 and 3. Both the instantaneous snapshots and time-averaged values are used to ascertain that the flame is statistically stable. In Sec. 4.4, in addition to the transport analyses used in the previous chapters, flame base propagation is also investigated to decide on the dominant flame stabilization mechanism. Finally, the findings are concluded in Sec. 4.5.

4.2 Domain configuration

For the turbulent multi-jet flame case, the domain is constructed as a cuboid, as shown in Fig. 4.1. The burner configuration is chosen with the primary combustion chamber of a staged gas-turbine engine in mind, where the combustion occurs under rich conditions [84]. To achieve a relatively high jet Reynolds number for a feasible computational cost, the diameter of the jets is increased, resulting in a rich global equivalence ratio of ≈ 3.3 . In previous studies, the global equivalence ratio based on inflowing mixture conditions was ≈ 7.6 [47], ≈ 14.4 [14], and ≈ 3.0 [63] (when the ambient air velocity was estimated to be 0.1 m/s). Pure hydrogen is fed to the domain from the round jets located at the $x = 0$ boundary. Essentially, two complete jets enter the domain in total: one complete jet in the middle and four quarter jets centered at the corners (periodic boundaries).

The jets have a diameter of 2 mm and are surrounded by the co-flowing preheated oxidizer, which consists of 12% O_2 and 88% H_2O by mole. The fuel is issued into the domain from the jet exits at 288 K with a maximum inflow velocity of 210 m/s. The co-flowing oxidizer has a maximum temperature of 916.5 K and a maximum velocity of 15 m/s. The pressure is moderately elevated to 2 atm. The mean velocity and scalar profiles at the inlet are specified by the tangential profile defined in Sec. 3.2. The initial temperature field is depicted in Fig. 4.1. The distance between the jets in Planes I and II shown in Fig. 4.1 corresponds to L_y for Cases I and II.

The domain has dimensions $L_x \times L_y \times L_z = 21 \times 7 \times 7 \text{ mm}^3$ and is discretized using $N_x \times N_y \times N_z = 1820 \times 612 \times 612$ uniform mesh points. The number of mesh points is selected so that there are at least ten points across the reaction-zone thickness. The x -direction is defined as the streamwise direction, and the boundaries at $x = 0$ and $x = L_x$ are defined as inflow and outflow boundaries, respectively, specified using NSCBC [73]. All the other boundaries are specified as periodic boundaries. A homogeneous isotropic

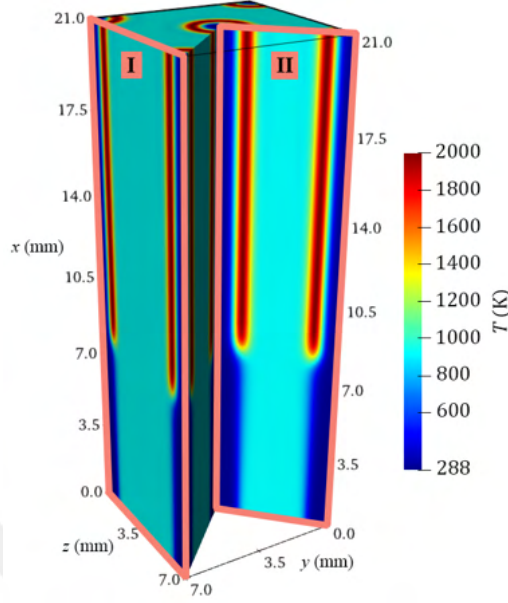


Figure 4.1: Initial temperature field for the 3D multi-jet configuration. Planes I and II correspond to the sample cross sections and are denoted by thick pink lines.

turbulence field is superimposed over the mean jet velocity, which is preliminarily determined using an incompressible DNS. The Reynolds number of the turbulence based on the Taylor microscale is 37.4, and the turbulence intensity is much smaller than that of the shear-generated turbulence in the combustion domain.

4.3 Structure of turbulent multi-jet flames

4.3.1 Large-scale flame structure

Instantaneous iso-surfaces of the stoichiometric mixture fraction ξ_{st} and the OH mass fraction corresponding to 5% of its maximum value in the domain ($Y_{OH} = Y_{OH,5\%}$), colored by temperature, are depicted in Fig. 4.2. The instantaneous snapshots are taken at $t = 1.15$ ms, which is equivalent to 11.5 flow-through times (τ_f). Figure 4.2 shows that both the ξ_{st} and Y_{OH}

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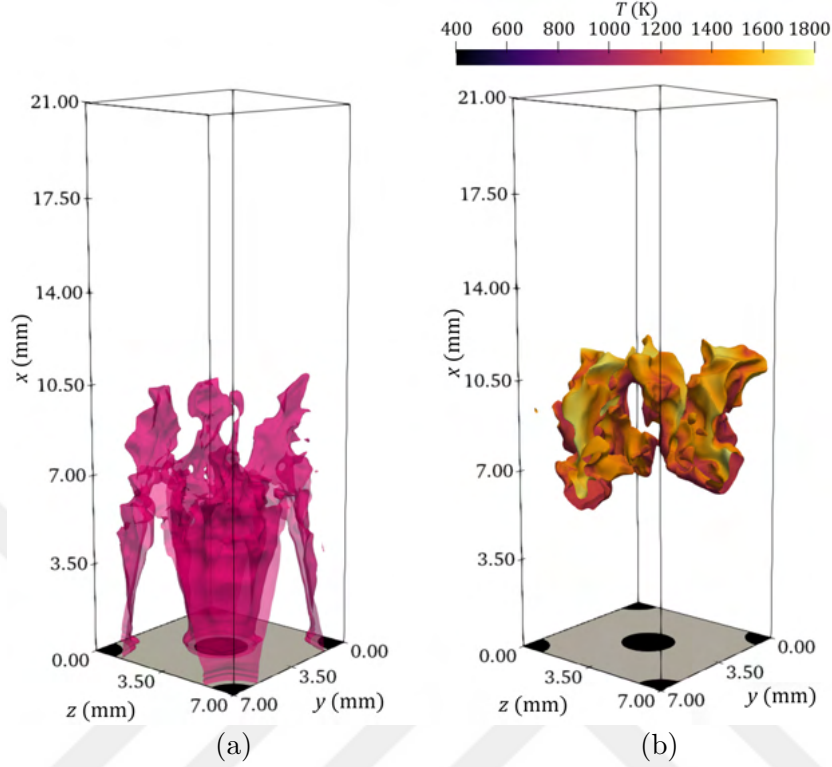


Figure 4.2: The instantaneous iso-surfaces of (a) the stoichiometric mixture fraction and (b) 5% of the maximum Y_{OH} , colored by temperature.

iso-surfaces of the jets from multiple burners merge. This behavior is similar to that seen for Case II but was not observed in the previous studies of turbulent single lifted-jet flames [14, 16, 47, 48, 51, 63, 64]. The merging of the stoichiometric iso-surfaces happens in the oxidizer side, leaving rich mixtures downstream.

In the presence of turbulence, both the ξ_{st} and Y_{OH} iso-surfaces (Figs. 4.2a and 4.2b) are highly complex. Using a single scalar to define the flame base, as in Refs. [47, 61, 76], could be inappropriate under such large scalar fluctuations. Therefore, following previous studies [15, 16, 85, 86], the flame base is defined using a more rigorous approach involving a second scalar. The quantity ξ is chosen as the second scalar, and the intersection between the ξ_{st} and $Y_{OH,5\%}$ iso-surfaces is defined as the flame base.

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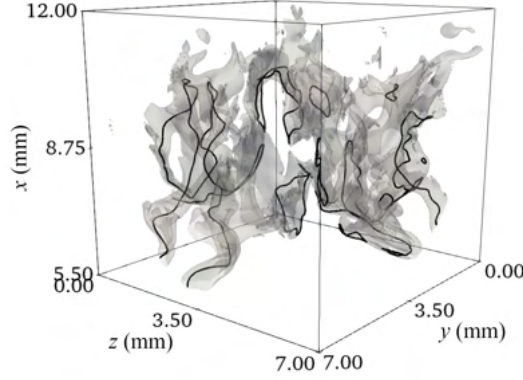


Figure 4.3: The instantaneous flame-base locations (solid black lines), and the flame-base region ($\dot{Q} \geq 0.3\dot{Q}_{max}$).

In Fig. 4.3, the solid black lines indicate the flame-base locations identified by the intersections, and the transparent gray iso-surface corresponds to the flame-base region ($\dot{Q} \geq 0.3\dot{Q}_{max}$). Given that the intersections closely coincide with the flame-base region, the flame base is well represented by the chosen scalars even for an interacting lifted flame resulting from the multi-jet configuration. The flame-base locations and flame-base regions are visualized over $\sim 2.4\tau_f$, and it is observed that the flame-base locations remain close to the flame-base regions at all times.

The most important difference between the turbulent and laminar multi-jet flames is that the former results in a single connected flame-base region. This behavior can be clearly seen in Figs. 4.4b and 4.4c. However, if the laminar multi-jet flames (Fig. 3.2a and 3.2b) were interpreted in a 3D space, the two flame-base regions would be extended around the jet-center axes, resulting in two disconnected flame-base regions. Note that for the laminar multi-jet flame cases, the jet centers are located at $y = 0$ and $y = L_y$, contrary to the well-accepted configuration of a single-jet lifted flame.

Figure 4.3 shows that the flame-base region is highly complex, especially in the streamwise direction, resulting in an almost $16\delta_L$ difference between

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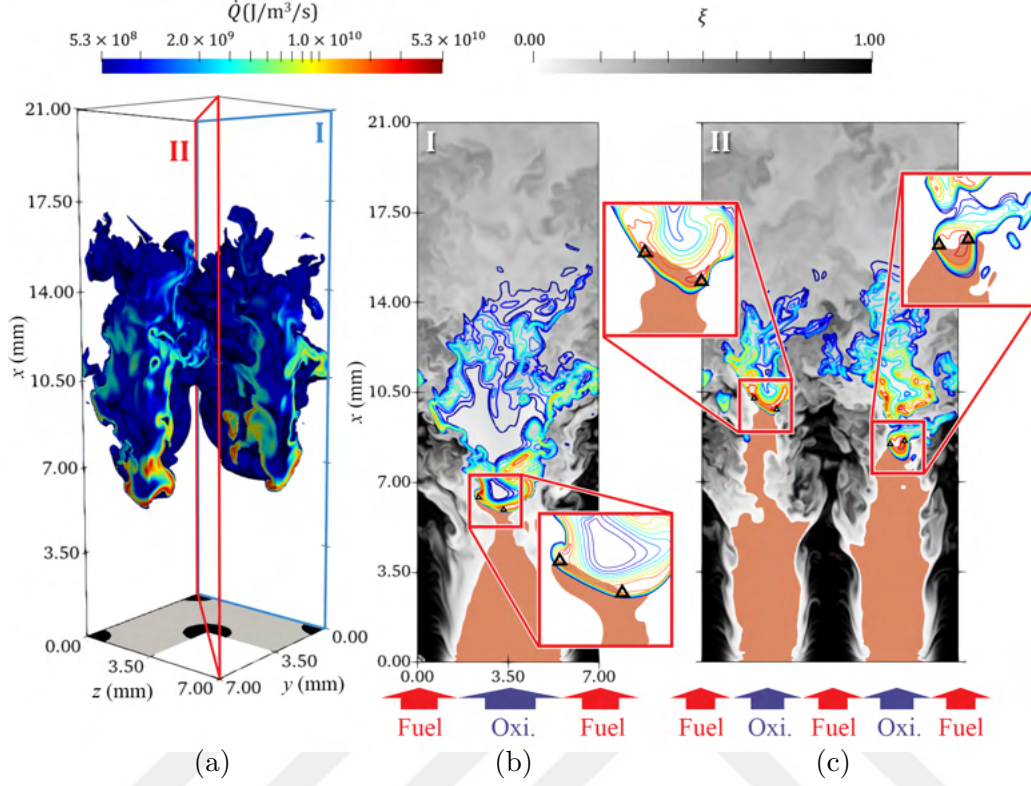


Figure 4.4: Instantaneous contours of substantial heat-release rate (a), and ξ contours superimposed by iso-lines of substantial heat-release rate on the $y = 0$ plane (b) and on the diagonal plane along $y = z$ (c). The $y = 0$ and diagonal planes are marked as Planes I and II, respectively. The orange regions represent the lean mixtures, and the flame-base locations are indicated by triangles. The magnified sections do not include the ξ contours for clarity.

the most-upstream and most-downstream flame-base locations. Here, δ_L is the laminar-flame thermal thickness for a stoichiometric mixture at a frozen mixing temperature.

The field of substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) is illustrated in Fig. 4.4 (where the color is on a logarithmic scale). As opposed to the $Y_{OH,5\%}$ iso-surface shown in Fig. 4.2b, the $\dot{Q}$ field provides insight into the downstream flame structure. In Fig. 4.4a, one-quarter of the $\dot{Q}$ field is removed to reveal the flame structure inside the reaction zones.

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Figures 4.4b and 4.4c show vertical slices of the mixture-fraction contours, superimposed by logarithmic heat-release rate iso-lines obtained from the $y = 0$ plane and the diagonal plane along $y = z$. Regions with a lean mixture fraction ($\xi < \xi_{st}$) are shaded in orange, and the outlines of these regions correspond to the ξ_{st} iso-lines. The flame-base locations are marked by triangles. The relationship between the flame structure and the merging ξ_{st} iso-surfaces is clear in Fig. 4.4b and 4.4c. The shaded lean-mixture regions show that the ξ_{st} iso-surfaces merge only around the flame-base locations, leaving a rich mixture fraction for the rest of the flame downstream. This behavior is clearly different from that of the laminar multi-jet flames. For Case II, the merging of the ξ_{st} iso-lines occurs approximately $26\delta_L$ downstream of the flame-base locations, and lean premixed flame branches are seen downstream of the flame-base region. This difference is possibly caused by the higher fuel-jet velocity for the turbulent multi-jet flames and the resulting turbulence, which increases the mixing of the scalars.

As clearly shown in Fig. 4.4b and 4.4c, the three-dimensionally connected region of high $\dot{Q}$ is located between the two neighboring jet streams, well outside the jet-core regions. This feature is not seen in single-burner turbulent lifted flames [47, 48, 63, 64], where the highest heat-release rate is usually observed for the rich premixed flame branch near the jet-core region.

The most-upstream flame-base locations are observed between the corner jets (on Plane I in Fig. 4.4b). By contrast, the most-downstream positions are seen between the central jet and the corner jets (on Plane II in Fig. 4.4c). It is interesting to note that although the distance between the jets is smaller for Plane II than for Plane I, the flame base associated with the jets is further downstream for Plane II than for Plane I.

To further analyze the structure of the turbulent multi-jet flames, the NFI defined in Sec. 2.4 is calculated. Figure 4.5a shows instantaneous NFI contours for regions with a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$). One-quarter of the domain is removed to visualize the inside of the reaction

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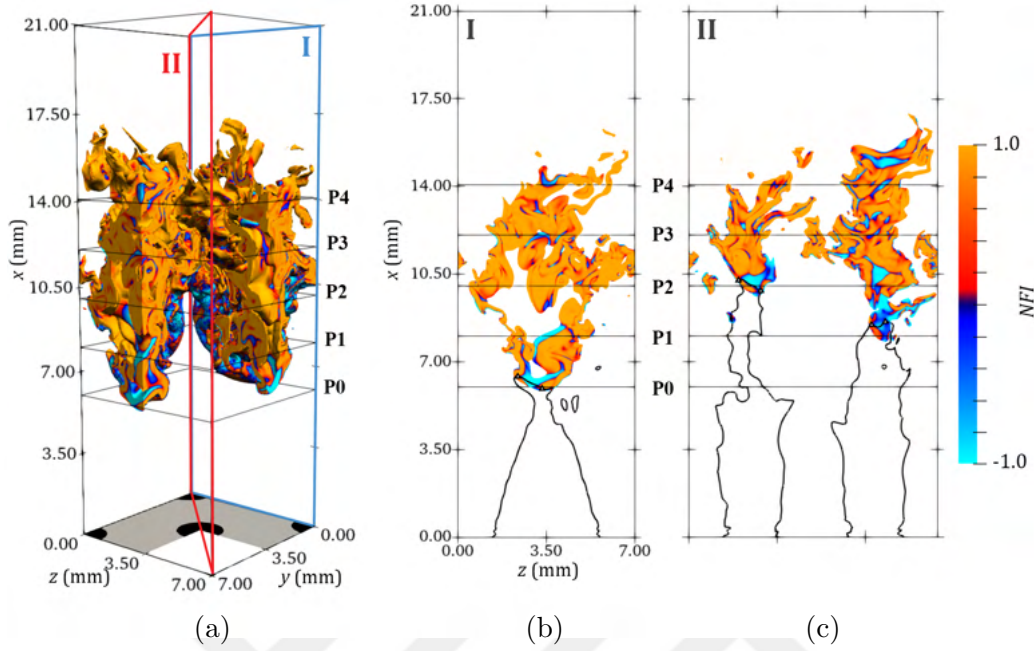


Figure 4.5: Instantaneous contours of the normalized flame index for regions with a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) in 3D space (a), at the $y = 0$ plane (b), and at the diagonal plane along $y = z$ (c). The $y = 0$ and diagonal planes are marked as Planes I and II, respectively. The black lines are ξ_{st} iso-lines, and the flame-base locations are marked by triangles.

zones. Slices on the $y = 0$ plane (Plane I) and the diagonal plane along $y = z$ (Plane II) are depicted in Figs. 4.5b and 4.5c, respectively. These figures show that the domain contains both premixed and diffusion flames. The diffusion flame branch occupies a much smaller volume than that for the laminar flames (Figs. 3.2e and 3.2f), leaving primarily premixed regions for the turbulent multi-jet flames.

Although Figs. 4.4 and 4.5 provide general insights into the instantaneous flame structure, more statistical analyses are needed to study the structure in detail. Similar to the analyses performed for the laminar flames in Fig. 3.3, conditional averages of the heat-release rate and the NFI on the mixture fraction, as well as the PDF of the mixture fraction, are calculated using 14 snapshots collected for $\sim 2.4\tau_f$. Only the regions with a substantial heat-

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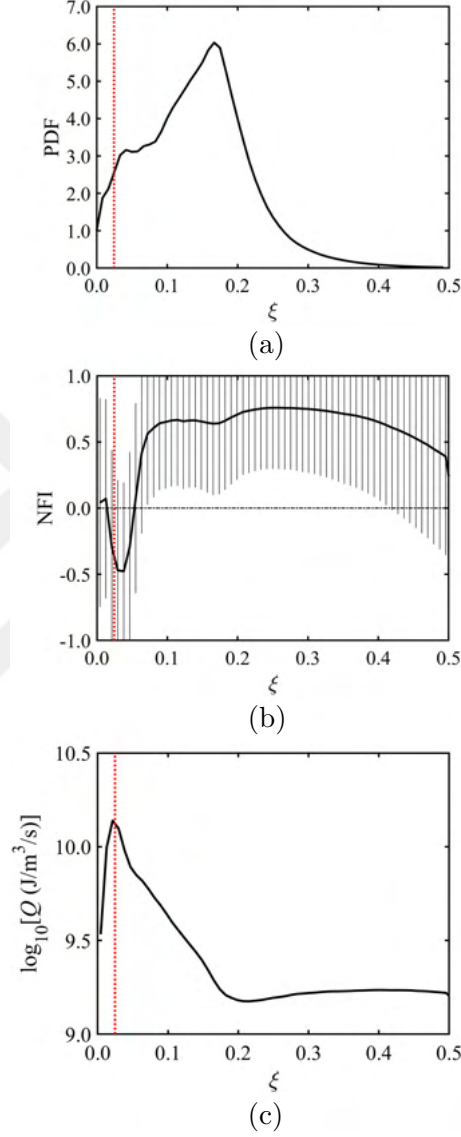


Figure 4.6: PDF of mixture fraction (ξ) (a), and average values of the normalized flame index (NFI) (b) and heat-release rate ($\dot{Q}$) (c) conditioned on ξ for the turbulent case. The vertical lines correspond to ξ_{st} . Only samples that have a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) are used.

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release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) are included in the analyses, and the results are illustrated in Fig. 4.6.

Figure 4.6a shows that the mixture fraction is broadly distributed on the rich side in contrast to the laminar-flame results (Fig. 3.3a). However, this behavior is expected for turbulent multi-jet flames because the merging of the ξ_{st} iso-surfaces occurs only downstream of the flame-base locations, leaving a rich premixed flame for the downstream reaction zones, as discussed above. As illustrated in Fig. 4.6b, the most intense reaction zones yield $-0.5 < NFI < 0.5$ over a range of ξ values on average, with a large standard deviation. This observation suggests that premixed and diffusion mixing modes co-exist, as seen in the instantaneous NFI field in Fig. 4.5.

In the lean regions, the average NFI values are close to $NFI = 0$. This finding suggests that both lean premixed and diffusion flames exist in the lean regions and that neither one dominates the other in terms of occupied volume. Such behavior is somewhat different from the laminar-flame results (Fig. 3.3b). Around ξ_{st} , the average NFI values become negative, indicating the presence of diffusion flames. This observation is similar to that for the laminar flames and is consistent with the instantaneous snapshots in Fig. 4.5.

For fuel-rich regions, the mean NFI values remain positive, suggesting premixed flames. The conditional average of the heat-release rate on the mixture fraction in Fig. 4.6c has one distinct peak around ξ_{st} , which indicates that the highest average $\dot{Q}$ is produced in the mixture fractions around stoichiometry. A peak in the average $\dot{Q}$ around ξ_{st} is also observed for the laminar cases. However, the laminar flames exhibit a second peak at slightly rich ξ (Fig. 3.3c), whereas the rich mixtures in the turbulent flames yield no such second peak, and $\dot{Q}$ is smaller on average compared with the lean mixtures in the turbulent flames.

4.3.2 Spatial evolution of the flame structure

The visualizations of the instantaneous reaction zones and the time-averaged statistical analyses in Sec. 4.3.1 provide insight into the overall flame structure. However, local flame structures could be different for different streamwise distances. To clarify the evolution of the flame structure along the streamwise direction, variations in the y - z cross sections (P0 to P4) marked in Fig. 4.5 are investigated. Figure 4.7a shows contours for the instantaneous logarithmic heat-release rate and mixture fraction, and Fig. 4.7b depicts the NFI contours for the regions with a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$) in the y - z cross sections at different streamwise positions (P0 to P4). The first position (P0) corresponds to the most-upstream flame-base location at each snapshot, and the other positions (P1–P4) are separated by $8\delta_L$ from one another. The flame-base locations, corresponding to the intersections of the $Y_{OH,5\%}$ and ξ_{st} iso-contours, are marked by circles in Fig. 4.7a.

At P0, the reaction zones exist in a relatively small volume at approximately $z = 3.5$ mm. Figure 4.7a shows that these reaction zones are overall lean, and the highest heat-release rate is seen around the flame-base locations, similar to the laminar flames in Secs. 2.4 and 3.3. The NFI contours (Fig. 4.7b) at P0 indicate that most of the reaction zones consist of both lean premixed and diffusion flames, with a small volume of rich premixed flames.

At P1 and P2, the lean regions become smaller than those at P0, which implies that the reaction zones mainly contain rich mixtures. The heat-release rate iso-lines in Fig. 4.7a show that the regions with high $\dot{Q}$ at P1 and P2 occur in both lean and rich regions. The $\dot{Q}$ values are always high around the flame base locations, although not all high- $\dot{Q}$ regions are observed around these locations. The NFI contours in Fig. 4.7b suggest that large parts of the lean regions are premixed, and the diffusion flame is seen around the ξ_{st} iso-lines, similar to the laminar cases. However, after P0, most of the reaction zones consist of rich mixtures, unlike for the laminar flames.

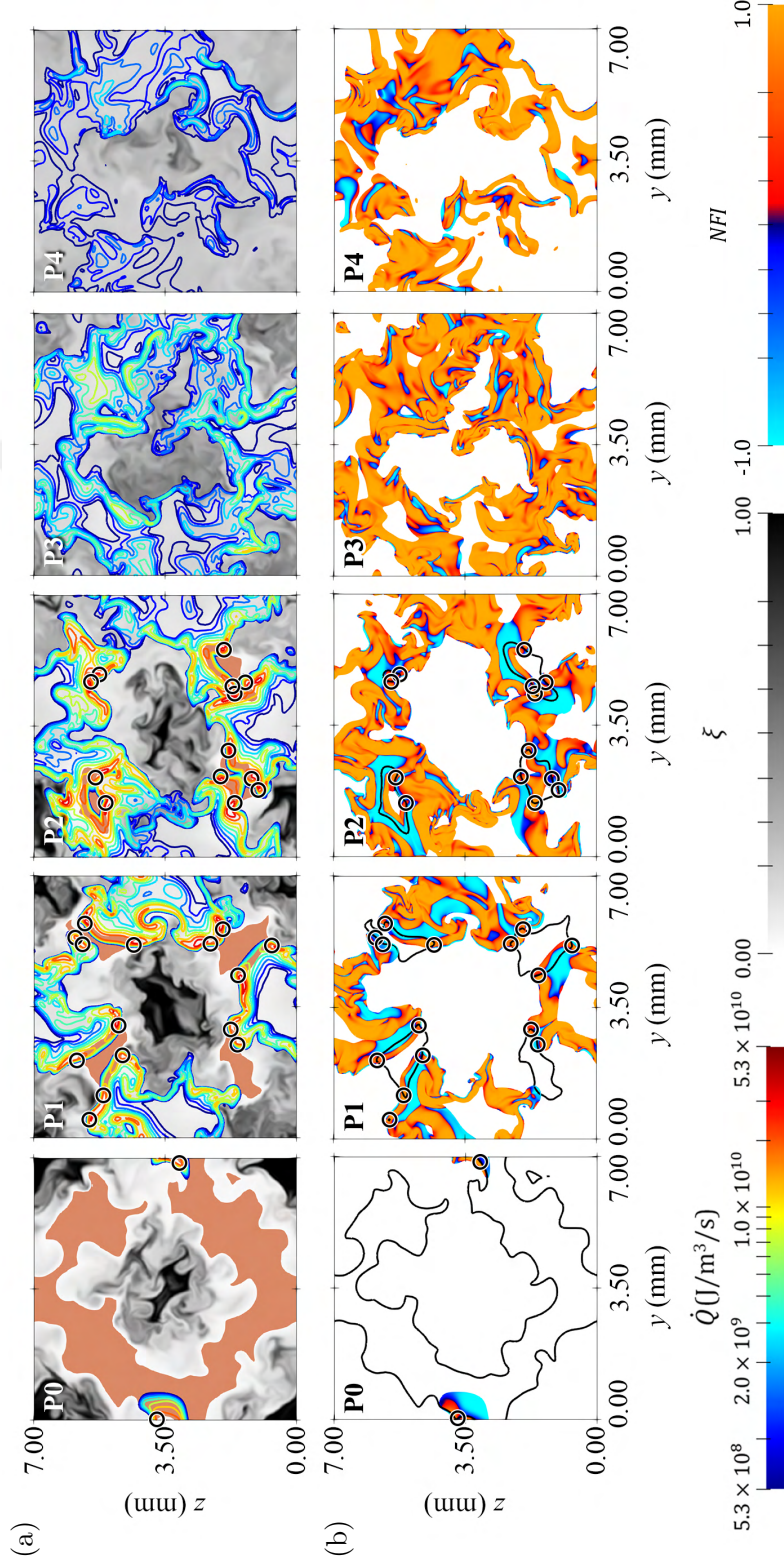


Figure 4.7: Instantaneous contours of (a) the mixture fraction superimposed by heat-release rate iso-lines (orange shading corresponds to lean regions) and (b) the normalized flame index (NFI) at regions with a substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$). The black lines are stoichiometric mixture fraction iso-lines, and the centers of the circles indicate the flame-base locations.

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Figure 4.7a indicates that the regions with an intense heat-release rate ($\dot{Q} > 2 \times 10^{10} \text{ J/m}^3/\text{s}$) existing around the flame-base locations for P0–P2 are not present for P3 and P4. The highest $\dot{Q}$ observed at P3 and P4 is an order of magnitude lower than that at P1 and P2. Moreover, the volume of the diffusion-flame regions becomes smaller with the increased mixing downstream. A visual inspection of the y - z planes at the different streamwise positions suggests that the tribrachial structure exists until P2, which is slightly downstream of the most-downstream flame-base location. After P2, the flame structure becomes premixed.

The average NFI and ξ , conditioned on the logarithm of the substantial heat-release rate ($\dot{Q} > 0.01\dot{Q}_{max}$), are calculated for 14 snapshots collected for $\sim 2.4\tau_f$ at the different streamwise positions (P0 to P4) and are depicted in Fig. 4.8.

Figure 4.8a illustrates the results for P0, which is the most-upstream flame-base location. The conditionally averaged mixture fraction shows that the reaction zones are lean overall at this position, consistent with a visual examination of Fig. 4.7. The NFI in Fig. 4.8a has negative values up to $\log_{10}[\dot{Q}(\text{J/m}^3/\text{s})] = 10$, which suggests that the mixture is overall non-premixed. For larger heat-release rates, the NFI values become positive, which indicates that premixed flames are responsible for the high heat-release rate around the most-upstream flame base.

P1 and P2 correspond to regions between the most-upstream and the most-downstream flame-base streamwise positions. The results of the statistical analyses conducted at P1 and P2 are shown in Fig. 4.8b. The NFI plot suggests that most of the reaction zones are premixed at P1 and P2, but the large standard deviation of the NFI suggests that the diffusion flame still exists. The conditional average of the mixture fraction in Fig. 4.8b shows that the mixture becomes overall rich at P1 and P2. However, the large standard deviation of ξ indicates that the lean premixed and diffusion flames are still present. This conclusion is consistent with the instantaneous fields

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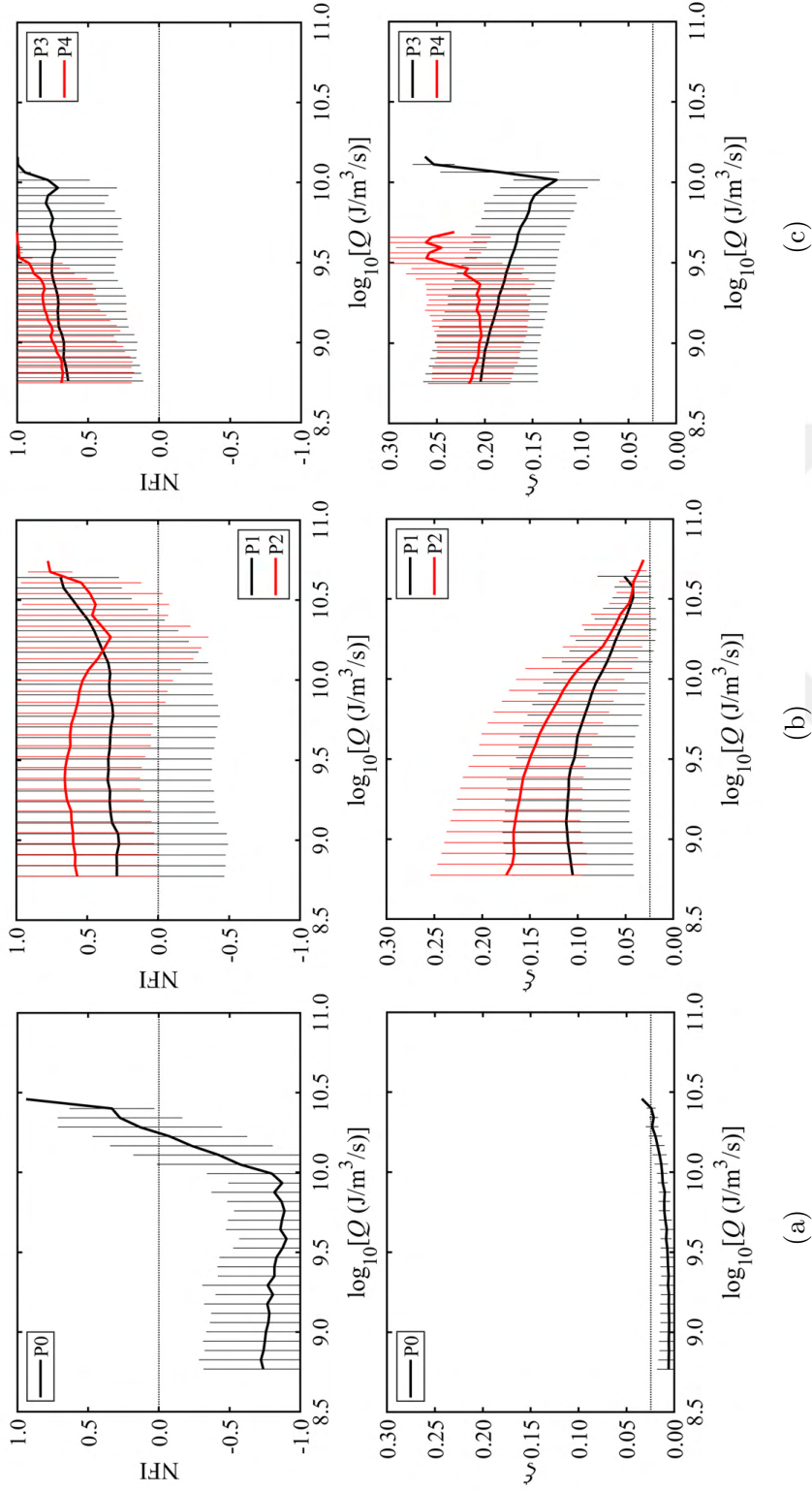


Figure 4.8: Mean values of the normalized flame index (NFI) and mixture fraction (ξ) conditioned on the logarithmic heat-release rate at (a) the most-upstream flame-base location, (b) cross sections up to the most-downstream flame base locations, and (c) locations further downstream. Samples are collected for 2.47_f . Only samples that have substantial heat-release rates ($\dot{Q} > 0.01\dot{Q}_{max}$) are used.

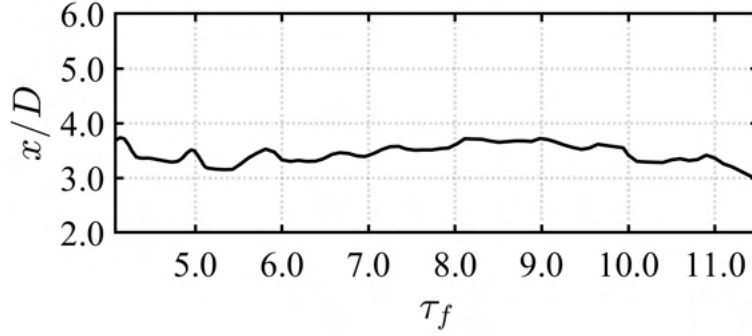


Figure 4.9: Temporal evolution of the most-upstream flame-base location in the streamwise direction.

shown in Fig. 4.7. The standard deviations of both the NFI and ξ decrease towards the regions with the highest heat-release rate, which demonstrates that this rate is produced by the slightly rich premixed flames. This feature is similar to the laminar case, where the highest $\dot{Q}$ is produced slightly on the rich side (See Figs. 3.2a and 3.2b).

Finally, Fig. 4.8c suggests that in the more-downstream positions (P3 and P4), the mixture becomes completely rich. Compared with the reaction zones at the more-upstream locations, the highest $\dot{Q}$ value is an order of magnitude smaller, as also shown in Fig. 4.7a.

4.4 Stabilization of turbulent multi-jet flames

4.4.1 Propagation of the flame base

In this subsection, the propagation of the turbulent multi-jet flames is examined to investigate flame stabilization. Figure 4.9 shows the temporal evolution of the most-upstream flame-base streamwise position. The flame-base location fluctuates within a distance equal to the jet diameter (D) after $4\tau_f$ for almost $8\tau_f$, which suggests that the flame is approximately stabilized.

Further investigations are needed to study the propagation of the entire flame base, which is highly complex in the streamwise direction. Following

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previous studies [15, 16, 85, 86], a coordinate system that moves with the flow velocity is defined to determine the flame-base propagation. Initially, unit normal vectors, in the directions of the iso-surface normals for the mixture fraction and OH mass fraction, are defined as follows:

$$\mathbf{N}_\xi = -\frac{\nabla \xi}{|\nabla \xi|}, \quad (4.1)$$

$$\mathbf{N}_{Y_{OH}} = -\frac{Y_{OH}}{|Y_{OH}|}. \quad (4.2)$$

Then, the unit normal vector $\mathbf{T}_1$ that is normal to both $\mathbf{N}_\xi$ and $\mathbf{N}_{Y_{OH}}$ is introduced. Finally, the vector $\mathbf{T}_2$ that is normal to $\mathbf{T}_1$ and tangential to the ξ iso-surface is defined. $\mathbf{T}_1$ and $\mathbf{T}_2$ are given by

$$\mathbf{T}_1 = \frac{\mathbf{N}_{Y_{OH}} \times \mathbf{N}_\xi}{|\mathbf{N}_{Y_{OH}} \times \mathbf{N}_\xi|}, \quad (4.3)$$

$$\mathbf{T}_2 = \frac{\mathbf{N}_\xi \times \mathbf{T}_1}{|\mathbf{N}_\xi \times \mathbf{T}_1|}. \quad (4.4)$$

To determine the propagation speed of the flame base, displacement speeds of the ξ_{st} and $Y_{OH,5\%}$ iso-surfaces are used. Following previous studies [16, 77, 85, 86, 87], these speeds are defined as

$$S_z = \frac{1}{\rho|\nabla \xi|} \left(-\frac{\partial}{\partial x_j} \left(\rho D_\xi \frac{\partial \xi}{\partial x_j} \right) \right), \quad (4.5)$$

$$S_d = \frac{1}{\rho|\nabla Y_{OH}|} \left(-\dot{\omega}_{OH} - \frac{\partial}{\partial x_j} \left(\rho D_{OH} \frac{\partial Y_{OH}}{\partial x_j} \right) \right), \quad (4.6)$$

where $D_\xi = \lambda/\rho c_p$ is the local thermal diffusivity and D_{OH} is the local mass diffusivity of OH. The displacement speeds S_z and S_d are in the direction of the normal vectors of the ξ and Y_{OH} iso-surfaces, respectively. Then, using the defined coordinate system, the flame-edge displacement speed ($\mathbf{V}_e$) is computed as

$$\mathbf{V}_e = S_z \mathbf{N}_\xi + S_e \mathbf{T}_2. \quad (4.7)$$

Figure 4.10 provides a schematic of the flame base and the orientation of the flame-base displacement speed. S_e is the projection of $\mathbf{V}_e$ on the ξ

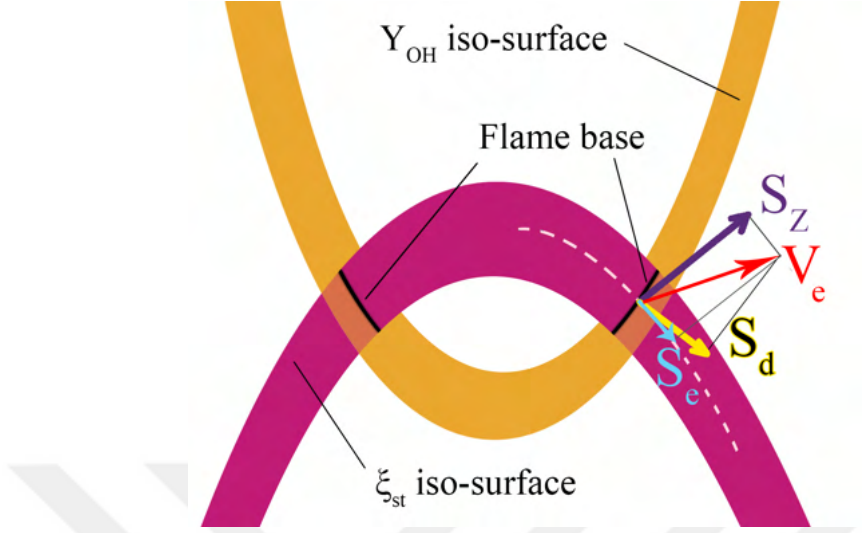


Figure 4.10: Schematic of the flame base, showing the orientations of the flame-base speeds.

iso-surface in the direction towards the reactant region. Using the vector components and Eqs. (4.5) and (4.6), S_e can be found as [16]

$$S_e = \frac{S_d - (N_{Y_{OH}} \cdot N_{\xi})S_z}{\sqrt{1 - (N_{Y_{OH}} \cdot N_{\xi})^2}}. \quad (4.8)$$

Figure 4.11 shows the JPDF and mean total flame-base velocity at the flame base positions of the turbulent jet flames, in the direction of $S_e \mathbf{T}_2$. The samples are collected over $\sim 2.4\tau_f$. The total flame-base velocity takes into account the velocity of the incoming flow. This incoming flow velocity, in the direction of $S_e \mathbf{T}_2$, is simply calculated as

$$u_e = \mathbf{u} \cdot \mathbf{T}_2. \quad (4.9)$$

The total flame-base velocity ($S_e + u_e$) is normalized by the flame-base displacement speed for Case I ($S_{d,I}$). Note that the S_d values for Case I and Case II ($S_{d,II}$) are similar ($S_{d,I} = 6.95\text{m/s}$, $S_{d,II} = 6.68\text{m/s}$), and $S_{d,I}$ is chosen arbitrarily as the reference laminar value. The JPDF distribution in Fig. 4.11 shows significant fluctuations for the total flame-base velocity. Nevertheless, the mean values of the total flame-base velocity conditioned on

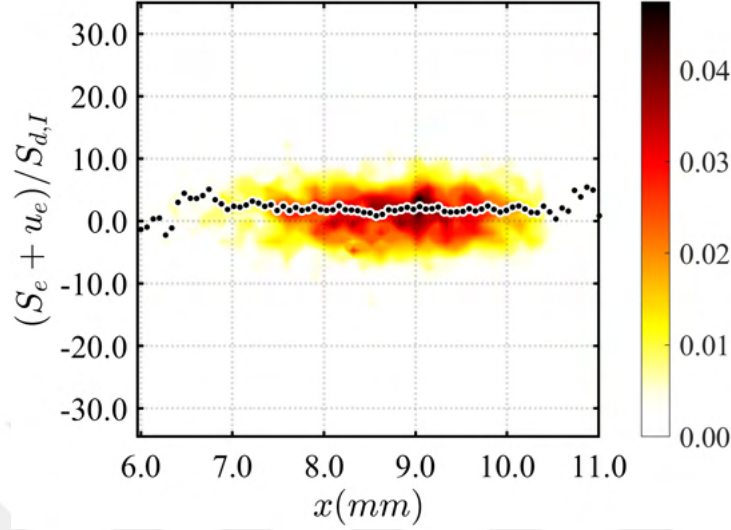


Figure 4.11: JPDF of the total flame-base velocity ($S_e + u_e$) and streamwise position, x . The dotted line represents the mean total flame-base velocity conditioned on x . $S_e + u_e$ is normalized by the flame-base displacement speed for Case I.

x are close to zero, suggesting that the flame propagation speed is balanced by the flow velocity, regardless of the streamwise location of the flame base. This result suggests that the flame base propagation plays an important role in the stabilization of the turbulent multi-jet flame.

4.4.2 Scalar dissipation rate

Scalar dissipation rate (χ) represents the rate of molecular scalar mixing [59], and it is a key parameter of non-premixed flames. If the χ exceeds the extinction limit (χ_e), the flame is quenched. In such case, the scalar dissipation has an important effect on determining the stabilization mechanism. In this study, the scalar dissipation rate is defined as the following, based on Refs. [88, 89]:

$$\chi = 2D_{th}(\nabla\xi)^2. \quad (4.10)$$

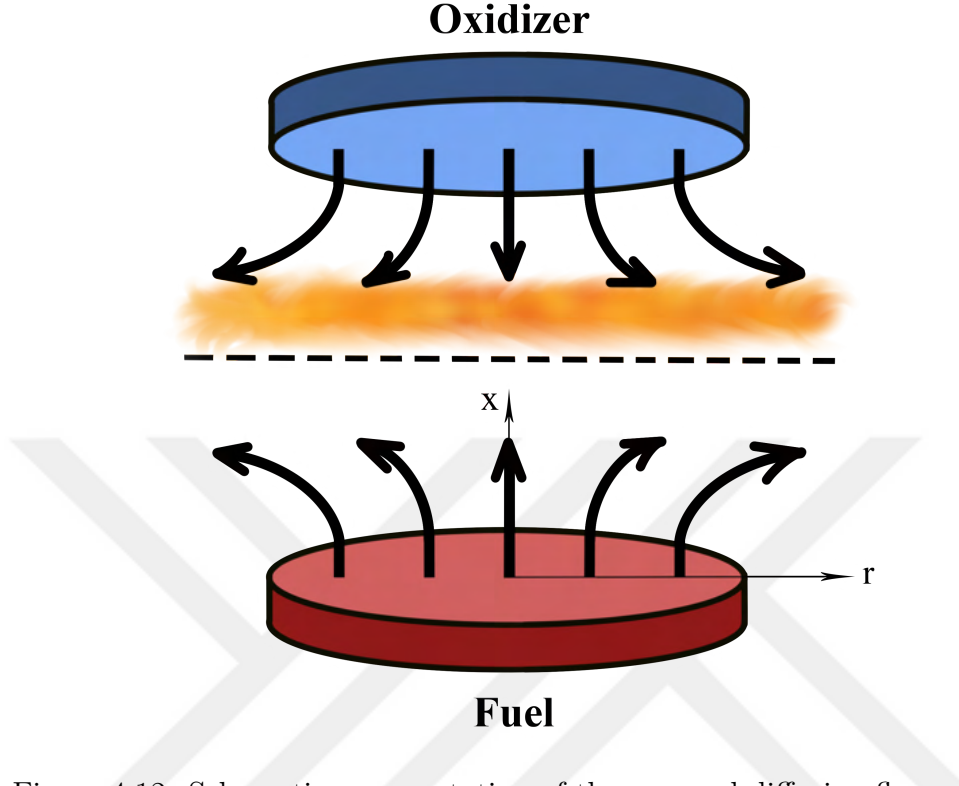


Figure 4.12: Schematic representation of the opposed-diffusion flame configuration.

In Eq. 4.10, D_{th} is the local thermal diffusivity, defined as

$$D_{th} = \lambda / \rho c_p, \quad (4.11)$$

where ρ , λ , and c_p correspond to mixture density, conductivity, and heat capacity, respectively.

The extinction scalar dissipation rate is calculated using the Flame Extinction Simulator of CHEMKIN-PRO. This simulator uses a series of iterations of opposed-flow simulations to determine the extinction strain rate of non-premixed flames [90]. The opposed-flow flame model computes a steady state solution for axisymmetric diffusion flames between two opposing nozzles, as depicted in Fig. 4.12. CHEMKIN-PRO uses the opposed-flame model originally developed by Kee *et al.* [91] for premixed flames, and the reduc-

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tion of 3D stagnation flow to 1D flow is based on von Karman's similarity solutions for incompressible flows [92].

The conservation of mass in cylindrical coordinates at steady state can be written as

$$\frac{\partial(\rho u)}{\partial x} + \frac{1}{r} \frac{\partial(\rho v_r r)}{\partial r} = 0 \quad (4.12)$$

where ρ is the density, and u and v_r are the axial and radial velocity components.

von Karman identified that v_r/r and other variables should only be the functions of x [92]. Using this, following two functions can be defined as:

$$G(x) = -\frac{\rho v_r}{r}, \quad F(x) = \frac{\rho u}{2}. \quad (4.13)$$

Using these two functions, Eq. 4.12 becomes

$$G(x) = \frac{dF(x)}{dx}. \quad (4.14)$$

The perpendicular momentum equation is written as

$$H - 2 \frac{d}{dx} \left(\frac{FG}{\rho} \right) + \frac{nG^2}{\rho} + \frac{d}{dx} \left[\mu \frac{d}{dx} \left(\frac{G}{\rho} \right) \right] = 0, \quad (4.15)$$

where H is the eigenvalue, satisfying the perpendicular momentum equation (Eq. 4.15):

$$H = \frac{1}{r} \frac{\partial p}{\partial r} = \text{constant} \quad (4.16)$$

Conservation of energy and species are given by

$$\rho u \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) + \frac{\rho}{c_p} \sum_{k=1}^{N_s} c_{pk} Y_k V_k \frac{dT}{dx} + \frac{1}{c_p} \sum_{k=1}^{N_s} h_k \dot{\omega}_k + \frac{1}{c_p} \dot{Q}_{rad} = 0 \quad (4.17)$$

and

$$\rho u \frac{dY_k}{dx} + \frac{d}{dx} (\rho Y_k V_k) - \dot{\omega}_k W_k = 0 \quad (4.18)$$

respectively. $\dot{Q}_{rad}$ refers to the heat loss due to gas and particle radiation, W_k is the molecular mass, and V_k is the diffusion velocity of the species.

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The boundary conditions are set as

$$x = 0 : F = \frac{\rho_f u_f}{2}; G = 0; T = T_f; \rho u Y_k + \rho Y_k V_k = (\rho u Y_k)_f \quad (4.19)$$

$$x = L : F = \frac{\rho_o u_o}{2}; G = 0; T = T_o; \rho u Y_k + \rho Y_k V_k = (\rho u Y_k)_o, \quad (4.20)$$

where o and f refer to oxidizer and fuel streams, respectively.

The Flame Extinction Simulator solves the Eqns. 4.12-4.18, and determines the extinction strain rate (K_{ext}) for the non-premixed flame conditions through a series of iterations. In this study, a two-point control is used to obtain the solutions. This method specifies the temperature at one point on both the oxidizer and the fuel sides. The varied flame strain rate (K) results in an S-curve for the maximum temperature (T_{max}) and strain rate plot. The turning point of this plot is interpreted as the extinction point. The extinction strain rate at this solution point is defined as the maximum axial flow velocity gradient on the fuel side just before the flame. CHEMKIN-PRO does not calculate the extinction scalar dissipation rate (χ_e) directly. However, using the K_{ext} definition, in this study, χ_e is defined as the maximum χ at the turning point solution. χ is calculated using the Eq. 4.10. The nozzle separation is set to 1.4 cm, and the fuel and oxidizer stream conditions are set as the same conditions as the turbulent multijet flame. The initial conditions for oxidizer and fuel streams of the opposed-flow flame simulations are summarized in Table 4.1.

Figure 4.13 shows the T_{max} as a function of K_{ext} . The S-curve of the flame response shows a turning point at the extinction strain rate around 60000 1/s. The strain rate at this solution point is calculated as $|dU/dx|$, and shown in Fig. 4.14. The extinction strain rate is defined as the maximum value of K , and the corresponds to 60000 1/s in Fig. 4.14, verifying the result observed in Fig. 4.13. The scalar dissipation rate at this point is also calculated using the Eq. 4.10, and the results are presented in Fig. 4.15. Following this figure, the χ_e is defined as the maximum χ at the extinction point, which corresponds to 15000 1/s.

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Table 4.1: Initial conditions set for the flame extinction analyses. Subscripts o and f refer to oxidizer and fuel streams, respectively.

Pressure	2 atm
Nozzle separation	1.4 cm
T_f	288 K
T_o	916.5 K
V_f	80 cm/s
V_o	80 cm/s
X_f	100% H_2
X_o	12% O_2 + 88% H_2O

Figure 4.16 shows the joint probability density function (JPDF) of S_e and the scalar dissipation rate (χ) at the flame-base positions of the turbulent multi-jet flames. The conditional mean of S_e is superimposed on this JPDF. The samples are collected at the flame-base locations over $\sim 2.4\tau_f$. The displacement speed is normalized by the flame-base displacement speed for Case I ($S_{d,I}$), and the scalar dissipation rate is normalized by the extinction flame dissipation rate. The highest probability of S_e is observed around $S_e = S_{d,I}$, which suggests that the most probable flame-base propagation speed for the turbulent case is comparable to that for the laminar cases. The distribution of S_e has a negative correlation with χ , which was previously observed for stabilized lifted flames [15, 86, 93, 94]. Figure 4.16 shows that the χ values at the flame base locations are significantly lower than the extinction scalar dissipation rate.

Low χ values at the flame base locations result from the unique flame structure of the turbulent multi-jet flames. As previously mentioned in Sec. 4.3.1, the flame base locations occur well outside the jet-core regions, whereas the highest scalar dissipation rate is observed around the jet-core. This can be seen in Fig. 4.17. The χ values around the flame base positions are significantly lower than the extinction scalar dissipation rate. Low χ values at the flame base suggest that the critical dissipation rate does not contribute to the stabilization of the turbulent multi-jet.

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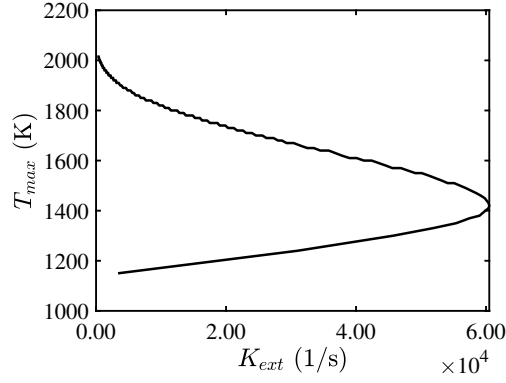


Figure 4.13: Flame response curve for the non-premixed flame of H_2 and O_2 diluted with H_2O .

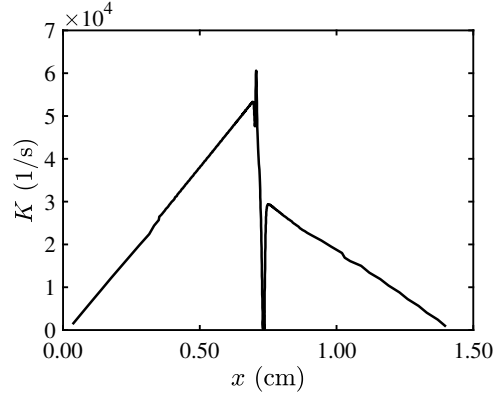


Figure 4.14: The strain rate for the non-premixed flame of H_2 and O_2 diluted with H_2O at the extinction point.

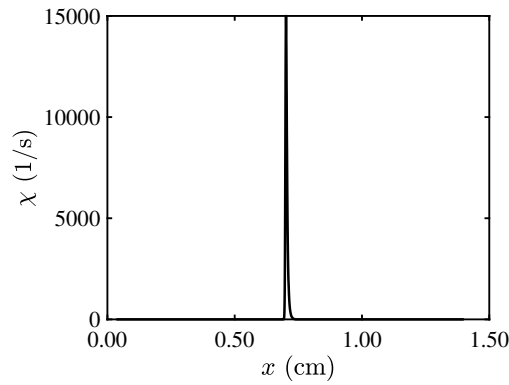


Figure 4.15: The scalar dissipation rate for the non-premixed flame of H_2 and O_2 diluted with H_2O at the extinction point.

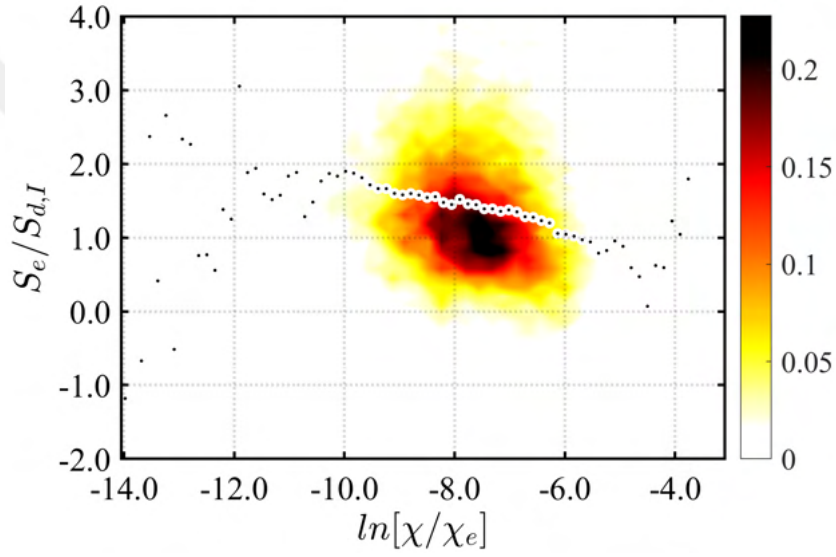


Figure 4.16: JPDF of the displacement velocity (S_e) and scalar dissipation rate χ at the flame base of turbulent multi-jet flames. The mean S_e conditioned on χ is shown by the dotted line. S_e is normalized by the flame-base displacement speed for Case I, and χ is normalized by the extinction scalar dissipation rate (χ_e).

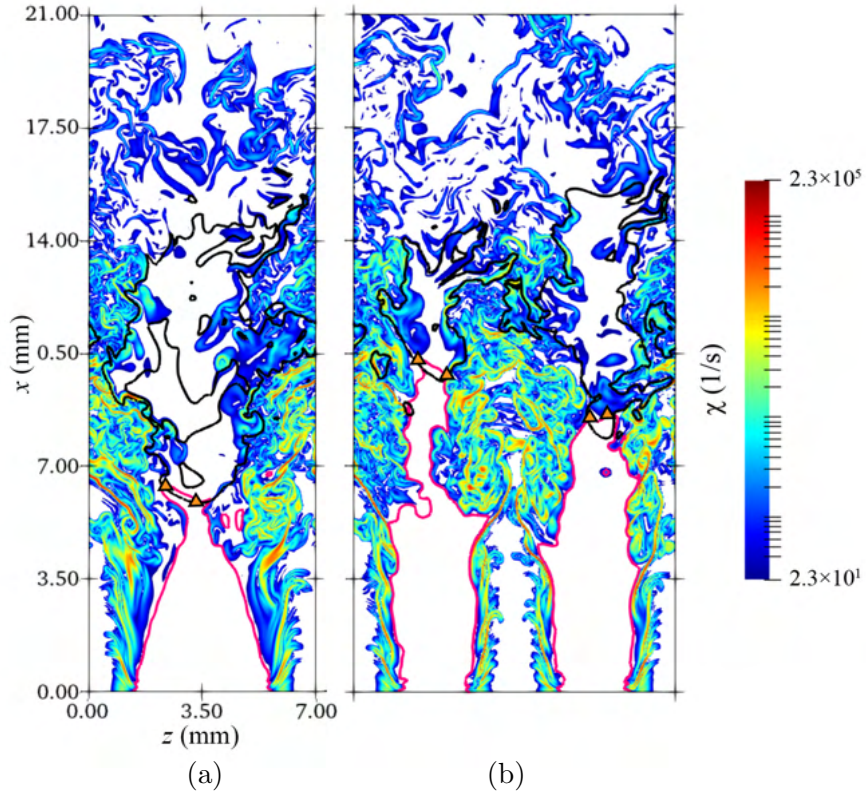


Figure 4.17: Instantaneous scalar dissipation rate contours at the $y = 0$ plane (a) and the diagonal plane along $y = z$ (b). The black lines are $\dot{Q} = 0.01 \dot{Q}_{max}$ iso-lines and pink lines are ξ_{st} iso-lines. Flame-base locations are marked by triangles.

4.4.3 Transport budget analysis

The results of Sec. 4.4.1 showed that the flame propagation velocity is balanced by the local flow velocity, suggesting that the flame propagation stabilization mechanism stabilizes the flame. In this section, this possibility is further investigated by using transport budget analysis.

In previous chapters, transport budgets were calculated along the ξ_{st} iso-lines. However, a more intricate approach is needed for the turbulent multi-jet flame with a complex flame base structure. Therefore, the coordinate system introduced in Sec. 4.4.1 is used for the transport budget analysis as well. $\mathbf{T}_2$ vector, which lies along the ξ_{st} iso-surface, in the direction of edge propagation, is used to evaluate the transport budget analysis. First, the budget terms and $\mathbf{T}_2$ are calculated for each flame base location. Then, a step is taken along $\mathbf{T}_2$, and budget terms and $\mathbf{T}_2$ is calculated at that position as well. This procedure is repeated for 50 steps and a distance of one δ_L in each direction. The path along $\mathbf{T}_2$ is shown schematically with a dashed line in Fig. 4.10.

Figure 4.18 shows the transport budget analysis of OH for the turbulent and laminar multi-jet cases. Since the transport budgets for the Case I and Case II were similar to each other, only Case I results are shown in Fig. 4.18 for simplicity. The transport terms of the turbulent case are averaged over all samples, conditioned on temperature. The averaged values of transport terms for the turbulent multi-jet flame show a similar trend to the laminar flames for the upstream of the reaction zone. The D-term, which is compatible with the R-term in magnitude, transports the OH species upstream of the reaction zone, accelerating the combustion in the upstream regions, and consequently, propagating the reaction zones. This result also supports that the flame is stabilized by the flame propagation mechanism.

A slight increase in the magnitude of the transport terms is observed in the downstream reaction zones. This difference suggests that the turbulence

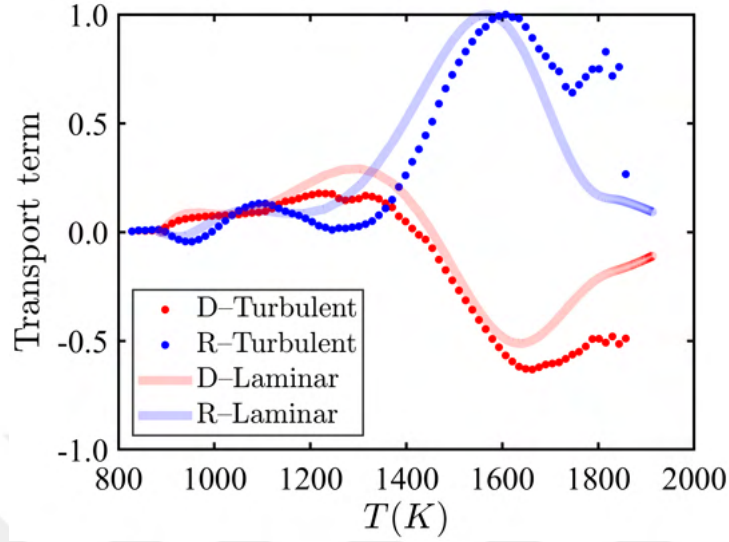


Figure 4.18: Transport budget analysis of OH for turbulent and laminar multi-jet flames. Transport terms are normalized by the maximum value of R-term for each case.

increases the diffusion of the species in the downstream reaction zones. The increased diffusion transport more species in these regions, resulting in an increase in the reaction term as well. However, this difference does not have an effect on the stabilization mechanism.

4.5 Interim conclusions

Direct numerical simulation of turbulent multi-jet flames is discussed based on the insights obtained for the laminar multi-jet flames. The distribution of the heat-release rate and the flame-base locations suggest that the turbulent flames, unlike the laminar ones, have a single connected flame-base region. This connected region has large fluctuations ($\sim 16\delta_L$) in its position in the streamwise direction. The highest heat-release rate is observed in the region farthest from the jet center, unlike typical single-jet lifted flames, where the maximum heat-release rate is seen well within the jet-core region. The NFI distributions suggest that the tribrachial structure is only observed around the flame base locations, and the merge of the ξ_{st} iso-surfaces results in a primarily rich premixed flame structure for the rest of the flame.

The propagation characteristics of the turbulent-flame base show that the propagation velocity of the flame base is balanced by the local flow velocity, which is an indicator of the flame base propagation mechanism. Furthermore, scalar dissipation rate distribution at the flame base locations suggests that the unique flame structure of the turbulent multi-jet flames prevents the critical scalar-dissipation rate from assisting flame stabilization. Further investigation of the OH transport budget shows a similar trend to the laminar flames, supporting the flame propagation as the main stabilization mechanism.

Even though substantial differences in the characteristics of the flame-base regions of laminar and turbulent multi-jet flames are observed, investigation of the flame stabilization mechanism reveals that these differences do not greatly influence flame-base propagation, and the turbulent multi-jet flame is stabilized by the flame base propagation mechanism.

Chapter 5

Conclusions

In this study, the flame features of lifted jet flames of non-premixed hydrogen and steam-diluted oxygen are investigated using direct numerical simulations. This study focuses on the effects of steam dilution, multi-jet configuration, and turbulence on the structure and stabilization mechanisms of lifted flames. Additionally, the effect of pressure on the flame features is investigated to verify the use of moderate pressures in the 3D turbulent simulations.

The results and conclusions obtained in each chapter can be summarized as follows.

In Ch. 2, the effects of diluent and pressure on the structure and stabilization mechanism of the lifted flames are investigated using canonical 2D laminar half-jet DNS configuration. Their effects on the ignition characteristics are further elucidated using a 0D homogeneous gas reactor, and the following conclusions are obtained:

1. Both the H_2O diluted and N_2 diluted cases have the typical tribrachial flame structure.
2. Under the same thermochemical conditions, a steam diluted lifted flame can have a different stabilization mechanism than an N_2 diluted flame, even though the overall flame structures are similar.

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3. H_2O has different physical and chemical properties than N_2 , but the ignition characteristics are most significantly affected by the high efficiency factor of H_2O , compared with N_2 .
4. The ignition characteristics show a non-monotonic behavior with respect to pressure. Steam dilution shifts this non-monotonic curve to lower pressures, owing to its high efficiency factor.
5. 2D laminar DNS study of the steam diluted lifted flame at higher pressures (2-20 atm) show that neither the overall structure nor the stabilization mechanism of the flames is affected by the pressure.

In Ch. 3, laminar multi-jet flames are investigated to understand the effect of multiple flames and their possible interaction on the flame features without the influence of turbulence. Two different cases with different domain sizes are investigated to observe the effect of jet separation on the flame structure. The thermochemical conditions are set to be the same as the nominal gas turbine conditions, used in Ch. 2, and pressure is set to be 2 atm. The flame structure and stabilization mechanism are investigated similarly to Ch. 2, and the following results are obtained:

1. The typical tribrachial structure is observed for both cases. The statistical distributions of $\dot{Q}$ and NFI are similar to single lifted flames under the same conditions as well.
2. The diffusion flame and the lean premixed flame branches of the case with shorter jet separation distance merge with each other inside the domain, downstream the flame base regions.
3. Both cases stabilize with the flame propagation stabilization mechanism. The transport budgets of OH show similar trends with the single-jet flame under the same conditions.

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In Ch. 4, a turbulent 3D multi-jet case, having the same conditions as the laminar flames in Ch. 3 is investigated to observe the effect of turbulence on the multi-jet flame structure and stabilization mechanism. Obtained results are as follows:

1. A single connected flame base region with large fluctuations in the streamwise direction is observed.
2. Highest heat release rate is observed outside the jet core regions.
3. The tribrachial structure is observed in a small region around the flame base positions. The flame structure is overall rich premixed in the downstream regions.
4. The propagation velocity of the flame base is balanced by the local flow velocity.
5. The unique structure of turbulent multi-jet flame prevents critical scalar dissipation rate from assisting flame stabilization.
6. The transport budget analyses show a similar trend with the laminar cases, suggesting that the flame propagation stabilization mechanism is stabilizing the turbulent multi-jet flames.

The present results suggest that using steam as an oxidizer diluent, instead of the conventionally used N_2 may result in a change in the flame stabilization mechanism. Under the nominal gas turbine conditions used for this study, the lifted flames of H_2 and O_2 diluted with steam show a tribrachial structure that stabilizes with flame propagation mechanism. In the presence of multi-jets, the flame structure and stabilization mechanism stay similar, even though the interaction of the flames may result in the merge of certain flame branches. When turbulence is considered, the structure of flames becomes complex. The flame base positions are observed outside jet

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core regions, where the tribrachial structure is observed for a small region. The unconventional features of the multi-jet flame structure in a turbulent environment imply that results from 2D optical imaging of such flames need to be interpreted with caution. However, even though the flame structure shows substantial differences with the laminar cases, the flame stabilizes with the flame propagation mechanism. This suggests that the current models can straightforwardly be applied to multi-jet configurations.



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Appendix A

Direct numerical simulation

A.1 Governing equations for reacting flows

Governing equations for fully-compressible reacting flows of N_s species are the following equations of

- Conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (\text{A.1})$$

- Conservation of momentum

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla \cdot \mathbf{P} + \rho \sum_{i=1}^{N_s} Y_i \mathbf{f}_i, \quad (\text{A.2})$$

- Conservation of energy

$$\rho \frac{\partial e_t}{\partial t} + \rho \mathbf{u} \cdot (\nabla e_t) = -\nabla \cdot \mathbf{q} - \mathbf{P} : (\nabla \mathbf{u}) + \rho \sum_{i=1}^{N_s} Y_i \mathbf{f}_i \cdot \mathbf{V}_i, \quad (\text{A.3})$$

- Conservation of species

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = -\nabla \cdot (\rho Y_i \mathbf{V}_i) + \omega_i, \quad (\text{A.4})$$

and the following relations,

$$\sum_i^{N_s} Y_i = 1, \quad \sum_i^{N_s} Y_i \mathbf{V}_i = 0, \quad \sum_i^{N_s} \omega_i W_i = 0. \quad (\text{A.5})$$

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Here, ρ , $\mathbf{u}$, and e_t correspond to the density, flow velocity vector, and internal energy respectively. Y_i , $\mathbf{f}_i$, $\mathbf{V}_i$, ω_i , and W_i denote the mass fraction, external force, diffusion velocity, reaction rate, and molecular weight of the i -th species.

$\mathbf{P}$ is the stress tensor, and for a Newtonian fluid, it can be defined as

$$\mathbf{P} = \left[p + \left(\frac{2}{3}\mu - \kappa \right) (\nabla \cdot \mathbf{u}) \right] \mathbf{I} - \mu \left[(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T \right], \quad (\text{A.6})$$

where p , μ , κ , and $\mathbf{I}$ correspond to pressure, dynamic viscosity, bulk viscosity, and identity matrix, respectively.

In Eq. A.3, $\mathbf{q}$ corresponds to the heat flux and is given by

$$\mathbf{q} = -\lambda \nabla T + \rho \sum_{i=1}^{N_s} h_i Y_i \mathbf{V}_i + R^0 T \sum_{i=1}^{N_s} \sum_{j=1}^{N_s} \left(\frac{X_j D_{T,i}}{W_i D_{ij}} \right) (\mathbf{V}_i - \mathbf{V}_j) + \mathbf{q}_R, \quad (\text{A.7})$$

where λ , T , R^0 , D_T , and D denote the thermal conductivity, temperature, the universal gas constant, thermal diffusion coefficient, and binary diffusion coefficient, respectively. h_i , X_i , and W_i correspond to the enthalpy, mole fraction, and molecular weight of the i -th species.

$\mathbf{V}_i$ in Eq. A.7 corresponds to the diffusion velocity of the i -th species, and it can be derived from the following equation:

$$\begin{aligned} \nabla X_i &= \sum_{j=1}^{N_s} \left(\frac{X_i X_j}{D_{ij}} \right) (\mathbf{V}_j - \mathbf{V}_i) \\ &+ (Y_i - X_i) \frac{\nabla p}{p} + \frac{\rho}{p} \sum_{j=1}^{N_s} Y_i Y_j (\mathbf{f}_i - \mathbf{f}_j) \\ &+ \sum_{j=1}^{N_s} \left[\left(\frac{X_i X_j}{\rho D_{ij}} \right) \left(\frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i} \right) \right] \frac{\nabla T}{T}. \end{aligned} \quad (\text{A.8})$$

Other relations used to define temperature and pressure are as follows:

$$e_t = \sum_{i=1}^{N_s} h_i Y_i - \frac{p}{\rho}, \quad (\text{A.9})$$

$$h_i = \Delta h_i^0 + \int_{T_0}^T c_{p,i} dT, \quad (\text{A.10})$$

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and finally, the equation of state for multi component ideal gas;

$$p = \rho R^0 T \sum_{i=1}^{N_s} \left(\frac{Y_i}{W_i} \right). \quad (\text{A.11})$$

The assumptions made for the current DNS are the following.

- Negligible Soret effect

$$\sum_{j=1}^{N_s} \left[\left(\frac{X_i X_j}{\rho D_{ij}} \right) \left(\frac{D_{T,j}}{Y_j} - \frac{D_{T,i}}{Y_i} \right) \right] \frac{\nabla T}{T} = 0. \quad (\text{A.12})$$

- Negligible Dufour effect

$$R^0 T \sum_{i=1}^{N_s} \sum_{j=1}^{N_s} \left(\frac{X_j D_{T,i}}{W_i D_{ij}} \right) (\mathbf{V}_i - \mathbf{V}_j) = 0. \quad (\text{A.13})$$

- Negligible pressure gradient diffusion

$$(Y_i - X_i) \frac{\nabla p}{p} = 0. \quad (\text{A.14})$$

- Negligible bulk viscosity

$$\kappa = 0. \quad (\text{A.15})$$

- Negligible radiative heat transfer

$$\mathbf{q}_R = 0. \quad (\text{A.16})$$

Taking the above assumptions and the auxiliary relations into account, the governing equations can be rearranged in the conservative form as follows:

- Conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (\text{A.17})$$

- Conservation of momentum

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla \cdot \mathbf{P}, \quad (\text{A.18})$$

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- Conservation of energy

$$\begin{aligned} \frac{\partial(\rho T)}{\partial t} + \nabla \cdot (\rho \mathbf{u} T) &= \frac{1}{\bar{c}_v} \nabla \cdot (\lambda \nabla T) - \frac{1}{\bar{c}_v} \sum_{i=1}^{N_s} (\rho Y_i \mathbf{V}_i c_{p,i} \cdot \nabla T) \\ &\quad - \frac{T}{\bar{c}_v} \sum_{i=1}^{N_s} [R_i \nabla \cdot (\rho Y_i \mathbf{V}_i)] - \frac{1}{\bar{c}_v} \mathbf{P} : (\nabla \mathbf{u}) \\ &\quad - \frac{1}{\bar{c}_v} \sum_{i=1}^{N_s} (h_i \omega_i) + \frac{T}{\bar{c}_v} \sum_{i=1}^{N_s} (R_i \omega_i), \end{aligned} \quad (\text{A.19})$$

- Conservation of species

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_i) = -\nabla \cdot (\rho Y_i \mathbf{V}_i) + \omega_i. \quad (\text{A.20})$$

In Eq. (A.19), R_i denotes characteristic gas constant of the i -th species, and $\bar{c}_v$ is the mixture averaged specific heat capacity at a constant volume. They are given by

$$R_i = \frac{R^0}{W_i}, \quad \bar{c}_v = \sum_i^{N_s} c_{v,i} Y_i. \quad (\text{A.21})$$

The stress tensor $\mathbf{P}$ equation (Eq. A.6) becomes

$$\mathbf{P} = \left[p + \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \right] \mathbf{I} - \mu \left[(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T \right]. \quad (\text{A.22})$$

The ":" on the right hand side of Eq. A.19 denotes the double dot product of two matrices, and $\mathbf{P} : (\nabla \mathbf{u})$ term can be calculated as follows:

$$\mathbf{P} : (\nabla \mathbf{u}) = (\mathbf{P} \cdot \nabla) \cdot \mathbf{u} = \sum_i \sum_j p_{ij} \frac{\partial u_i}{\partial x_j}. \quad (\text{A.23})$$

The diffusion velocity of the i -th species ($\mathbf{V}_i$) is given by

$$\mathbf{V}_i = -\frac{1}{X_i} D_{im} \nabla X_i. \quad (\text{A.24})$$

D_{im} denotes the mixture diffusion coefficient for the i -th species, and it is obtained by using binary diffusion coefficients D_{ij} as follows:

$$D_{im} = -\frac{1 - Y_i}{\sum_{i \neq j}^{N_s} X_i / D_{ij}}. \quad (\text{A.25})$$

A.2 Chemical reactions

The forward and backward reactions of a general k set of reactions are given by

$$\sum_{i=1}^{N_s} \nu'_{i,k} X_i \rightleftharpoons \sum_{i=1}^{N_s} \nu''_{i,k} X_i, \quad (\text{A.26})$$

where $\nu'_{i,k}$ and $\nu''_{i,k}$ are the stoichiometric coefficient for the i -th species in the k -th elemental reaction, and N_r is the number of elemental reactions. The reaction rate of the i -th species ω_i is determined by

$$\omega_i = \sum_{k=1}^{N_r} (\nu''_{i,k} - \nu'_{i,k}) q_k, \quad (\text{A.27})$$

where q_k is the total rate of progress variable, which can be written as:

$$q_k = k_{f_k} \prod_{i=1}^{N_s} [X_i]^{\nu'_{i,k}} - k_{r_k} \prod_{i=1}^{N_s} [X_i]^{\nu''_{i,k}}. \quad (\text{A.28})$$

k_{f_k} and k_{r_k} in Eq. (A.28) corresponds to the forward and backward rate constants respectively, and k_{f_k} is assumed to follow the following Arrhenius temperature dependence equation:

$$k_{f_k} = A_k T^{\beta_k} \exp\left(\frac{-E_k}{R_c T}\right). \quad (\text{A.29})$$

Here, A_k , β_k , and E_k represent the pre-exponential factor, the temperature exponent, and the activation energy for each elemental reaction, respectively. R_c corresponds to the universal gas constant with the unit [cal/(K mol)].

The backward reaction rate coefficient, k_{r_k} , is obtained by

$$k_{r_k} = \left(\frac{k_{f_k}}{K_{c_k}} \right), \quad (\text{A.30})$$

where K_{c_k} denotes the equilibrium constant determined by

$$K_{c_k} = K_{p_k} \left(\frac{P_{atm}}{R^0 T} \right)^{\sum_{i=1}^{N_s} (\nu''_{i,k} - \nu'_{i,k})}. \quad (\text{A.31})$$

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Here, K_{P_k} corresponds to the equilibrium constant, and it is obtained by using the entropy and enthalpy of the k -th elemental reaction as follows:

$$K_{P_k} = \exp \left(\frac{\Delta S_k}{R^0} - \frac{\Delta H_k}{R^0 T} \right). \quad (\text{A.32})$$

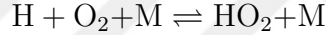
In the above equation, ΔS_k and ΔH_k are calculated as follows.

$$\frac{\Delta S_k}{R^0} = \sum_{i=1}^{N_s} (\nu''_{i,k} - \nu'_{i,k}) \frac{S_i}{R^0}, \quad (\text{A.33})$$

$$\frac{\Delta H_k}{R^0 T} = \sum_{i=1}^{N_s} (\nu''_{i,k} - \nu'_{i,k}) \frac{H_i}{R^0 T}. \quad (\text{A.34})$$

Three-body reactions

Some chemical reactions, such as the following, require a third body element to advance.



In such a case, the forward reaction rate q_k is calculated by considering the concentration of the third body element. Then, Eq. (A.28) becomes,

$$q_k = \left(\sum_{i=1}^{N_s} \alpha_{i,k} [X_i] \right) \left(k_{f_k} \prod_{i=1}^{N_s} [X_i]^{\nu'_{i,k}} - k_{r_k} \prod_{i=1}^{N_s} [X_i]^{\nu''_{i,k}} \right), \quad (\text{A.35})$$

where, $\alpha_{i,k}$ corresponds to the contribution of the third body element for the i -th species in the k -th elemental reaction. If all of the species contribute to the reaction equally as a third body, $\alpha_{i,k}$ becomes 1, which makes the first term in Eq. A.35 as follows:

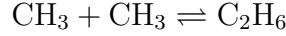
$$[M] = \sum_{i=1}^{N_s} [X_i]. \quad (\text{A.36})$$

However, in many cases, the contributions of the third body element of some species are higher than other species.

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Fall-off reactions

Under certain conditions, some reaction rate expressions depend on both temperature and pressure. Fall-off reactions are an example of such pressure-dependent reactions. The methyl recombination reaction is an example of the fall-off reactions. In the high-pressure limit, the reaction is described as:



On the other hand, in the low-pressure limit, a third-body element is needed to supply the energy to proceed the reaction, and the reaction is described as



for the low-pressure limit. This region is called as the fall-off region, and the reaction rate constants are in the Arrhenius form for the low pressure limit (k_0) and the high pressure limit (k_∞). The reaction rate constants at this region can be written as:

$$k_0 = A_0 T^{\beta_0} \exp\left(\frac{-E_0}{R_c T}\right), \quad (\text{A.37})$$

$$k_\infty = A_\infty T^{\beta_\infty} \exp\left(\frac{-E_\infty}{R_c T}\right). \quad (\text{A.38})$$

The reaction rate constant at any pressure is given by

$$k = k_\infty \left(\frac{P_r}{1 + P_r} \right) F, \quad (\text{A.39})$$

where, the reduced press P_r is given as,

$$P_r = \frac{k_0[M]}{k_\infty}. \quad (\text{A.40})$$

Here, $[M]$ is the molar concentration of the mixture and when $F = 1$, it becomes Lindemann form. In the present DNS, Troe form is adopted for the fall-off reactions in the chemical mechanism used, and F is given by

$$\log F = \left\{ 1 + \left[\frac{\log P_r + c}{n - d(\log P_r + c)} \right]^2 \right\}^{-1} \log F_{\text{cent}}. \quad (\text{A.41})$$

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The constants in the Eq. (A.41) are

$$c = -0.4 - 0.67 \log F_{\text{cent}}, \quad (\text{A.42})$$

$$n = 0.75 - 1.27 \log F_{\text{cent}}, \quad (\text{A.43})$$

$$d = 0.14. \quad (\text{A.44})$$

A.2.1 Thermodynamic properties

The temperature dependence of the thermodynamic and transport properties, namely viscosity, thermal conductivity and diffusion coefficient, are taken into account by using CHEMKIN-II packages [95, 96] with modifications for vector and parallel computation. this study considers the thermodynamic and transport properties as functions of temperature only, and the molar heat capacities at a constant pressure are given by polynomial fits:

$$\frac{C_{p,i}}{R^0} = \sum_{n=1}^N a_{n,i} T^{(n-1)}. \quad (\text{A.45})$$

The standard-state molar enthalpy is given by

$$H_i = \int_0^T C_{p,i} dT. \quad (\text{A.46})$$

Substituting Eq. (A.46) into Eq. (A.45), the following relation is obtained:

$$\frac{H_i}{R^0 T} = \sum_{i=1}^N \frac{a_{n,i} T^{(n-1)}}{n} + \frac{a_{N+1,i}}{T}. \quad (\text{A.47})$$

In the Eq. (A.47), the integrated constant $a_{N+1,i}$ corresponds to the standard enthalpy of formation at 0 K. However, since this representative polynomial is not valid near 0 K, $a_{N+1,i}$ is determined from the standard enthalpy of formation at 298 K, and therefore the enthalpy of the i -th species becomes:

$$H_i = \int_{298}^T C_{p,i} dT + H_i(298). \quad (\text{A.48})$$

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The entropy of each species at atmospheric pressure can be obtained by integrating the specific heat, and given as

$$S_i^0 = \int_0^T \frac{C_{p,i}}{T} dT. \quad (\text{A.49})$$

Substituting Eq. (A.49) into Eq. (A.45) gives

$$\frac{S_i^0}{R^0} = a_{1,i} \ln T + \sum_{n=2}^N \frac{a_{n,i} T^{(n-1)}}{n-1} + a_{N+2,i}. \quad (\text{A.50})$$

Similar to $a_{N+1,i}$, the integrated constant $a_{N+2,i}$ is determined by the standard enthalpy of formation at 298 K. $c_{p,i}$ and $\bar{c}_v$ in Eq. (A.19) are correlated to $C_{p,i}$ as follows:

$$c_{p,i} = C_{p,i}/W_i, \quad (\text{A.51})$$

$$C_{v,i} = C_{p,i} - R^0, \quad (\text{A.52})$$

$$c_{v,i} = C_{v,i}/W_i, \quad (\text{A.53})$$

$$\bar{c}_v = \sum_{i=1}^{N_s} c_v Y_i. \quad (\text{A.54})$$

A.2.2 Transport coefficients

The viscosity η_i , thermal conductivity λ_i and the binary diffusion coefficient D_{ij} for the i -th species are calculated by applying fitting procedure as a function of temperature T , and given as follows:

$$\ln \eta_i = \sum_{n=1}^N a_{n,i} (\ln T)^{n-1}, \quad (\text{A.55})$$

$$\ln \lambda_i = \sum_{n=1}^N b_{n,i} (\ln T)^{n-1}, \quad (\text{A.56})$$

$$\ln D_{ij} = \sum_{n=1}^N c_{n,i} (\ln T)^{n-1}. \quad (\text{A.57})$$

Here, the constants $a_{n,i}$, $b_{n,i}$ and $c_{n,i}$ are calculated until $N = 4$ by using TRANSPORT of CHEMKIN PACKAGE [96]. By using the calculated values

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of η_i , λ_i , D_{ij} , the following relations can be written:

$$\mu = \sum_{i=1}^{N_s} \frac{X_i \eta_i}{\sum_{j \neq i}^I X_j \Phi_{ij}}, \quad (\text{A.58})$$

$$\lambda = \frac{1}{2} \left(\sum_{i=1}^{N_s} X_i \lambda_i + \frac{1}{\sum_{i=1}^{N_s} X_i / \lambda_i} \right), \quad (\text{A.59})$$

$$D_{im} = \frac{\sum_{j \neq i}^{N_s} X_j W_j}{\overline{W} \sum_{j \neq i}^I X_j / D_{ij}}, \quad (\text{A.60})$$

where μ , λ , and D_{im} represent the viscosity, thermal conductivity, and the diffusivity of the i -th species in the multi component system. Φ_{ij} is given by

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_i}{W_j} \right)^{-\frac{1}{2}} \left\{ 1 + \left(\frac{\eta_i}{\eta_j} \right)^{\frac{1}{2}} \left(\frac{W_j}{W_i} \right)^{\frac{1}{4}} \right\}^2. \quad (\text{A.61})$$

A.3 Computational methods

A.3.1 Spatial discretization

The current DNS uses a fourth-order central finite difference scheme to discretize the governing equations in all directions. At a discretized point i , the partial derivatives of a function f_i with respect to x_k direction is given by:

$$\left(\frac{\partial f}{\partial x_k}\right)_i = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x_k} \quad (\text{A.62})$$

The derivatives at the domain boundaries can be written as:

$$\left(\frac{\partial f}{\partial x_k}\right)_1 = \frac{-25f_1 + 48f_2 - 36f_3 + 16f_4 - 3f_5}{12\Delta x_k}, \quad (\text{A.63})$$

$$\left(\frac{\partial f}{\partial x_k}\right)_2 = \frac{-3f_1 - 10f_2 + 18f_3 - 6f_4 + f_5}{12\Delta x_k}, \quad (\text{A.64})$$

$$\left(\frac{\partial f}{\partial x_k}\right)_{N_k-1} = \frac{3f_{N_k} + 10f_{N_k-1} - 18f_{N_k-2} + 6f_{N_k-3} - f_{N_k-4}}{12\Delta x_k}, \quad (\text{A.65})$$

$$\left(\frac{\partial f}{\partial x_k}\right)_{N_k} = \frac{25f_{N_k} - 48f_{N_k-1} + 36f_{N_k-2} - 16f_{N_k-3} + 3f_{N_k-4}}{12\Delta x_k}, \quad (\text{A.66})$$

where, N_k corresponds to the number of grid points in the x_k direction.

A.3.2 Spatial filtering

The numerical methods used for spatial discretization may cause unphysical oscillations with frequencies higher than the spatial resolution. An explicit spatial filter based on compact finite difference schemes [97] is applied to the density ρ , temperature (ρT), velocity components (ρu_i), and mass fraction ρY_i fields to eliminate these unphysical oscillations. The filtered

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values at node x_i ($\hat{f}_i$) is given by:

$$\hat{f}_i = af_i + \frac{d}{2}(f_{i+3} + f_{i-3}) + \frac{c}{2}(f_{i+2} + f_{i-2}) + \frac{b}{2}(f_{i+1} + f_{i-1}). \quad (\text{A.67})$$

The coefficients, a , b , c and d are determined by the matching Taylor series expansion coefficients. In this study, the sixth order explicit spatial filter is used, and therefore the coefficients a , b , c and d are determined as

$$a = \frac{11}{16}, \quad b = \frac{15}{32}, \quad c = -\frac{3}{16}, \quad d = \frac{1}{32} \quad (\text{A.68})$$

When the periodic boundary condition is not imposed on the domain boundaries, a fourth-order explicit filter, defined by the following equations, is applied near the domain boundaries.

$$\hat{f}_1 = \frac{15}{16}f_1 + \frac{1}{16}(4f_2 - 6f_3 + 4f_4 - f_5) \quad (\text{A.69})$$

$$\hat{f}_2 = \frac{3}{4}f_2 + \frac{1}{16}(f_1 + 6f_3 - 4f_4 + f_5) \quad (\text{A.70})$$

$$\hat{f}_3 = \frac{5}{8}f_3 + \frac{1}{16}(-f_1 + 4f_2 + 4f_4 - f_5) \quad (\text{A.71})$$

$$\hat{f}_{N_k-2} = \frac{5}{8}f_{N_k-2} + \frac{1}{16}(-f_{N_k} + 4f_{N_k-1} + 4f_{N_k-3} - f_{N_k-4}) \quad (\text{A.72})$$

$$\hat{f}_{N_k-1} = \frac{3}{4}f_{N_k-1} + \frac{1}{16}(f_{N_k} + 6f_{N_k-2} - 4f_{N_k-3} + f_{N_k-4}) \quad (\text{A.73})$$

$$\hat{f}_{N_k} = \frac{15}{16}f_{N_k} + \frac{1}{16}(4f_{N_k-1} - 6f_{N_k-2} + 4f_{N_k-3} - f_{N_k-4}) \quad (\text{A.74})$$

A.3.3 Boundary conditions

In the DNS of compressible reacting flows, the pressure waves are generated, and they propagate in a direction normal to the flame front at the speed of sound. If the periodic boundary conditions that are used for the DNS of non-reacting homogeneous isotropic turbulent flows are applied to the

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DNS of compressible reacting flows, the pressure waves will keep propagating throughout the domain, resulting in unphysical phenomena. Pressure waves may even be reflected from the zero gradient outflow boundary conditions. These unphysical reflections of waves, resulting from numerical methods used in the simulations, propagate through the domain, affecting the DNS results. In many cases, the reflected waves are offset by the numerical viscosity of the numerical schemes. Nevertheless, if a high order difference scheme is used for a high-resolution DNS, the numerical viscosity becomes very small, and the propagation of the reflected waves from the boundaries affects the reliability of the DNS results.

For the reasons mentioned earlier, Thompson [98] has applied non-reflecting conditions to the Euler equations by suppressing the amplitude of reflected waves with characteristic wave analysis. Later on, Poinso *et al.* [73, 99] extended the boundary conditions to the Navier–Stokes equations and named as the Navier–Stokes Characteristic Boundary Conditions (NSCBC). NSCBC is widely used in the numerical studies of compressible viscous flows to define the boundary conditions.

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Governing equations of NSCBC

At the boundary in the x -direction, the governing equations for NSCBC can be written as follows.

$$\frac{\partial \rho}{\partial t} + d_1 + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0, \quad (\text{A.75})$$

$$\frac{\partial \rho u}{\partial t} + u d_1 + \rho d_3 + \frac{\partial \rho u v}{\partial y} + \frac{\partial \rho u w}{\partial z} = \frac{\partial \tau_{1j}}{\partial x_j}, \quad (\text{A.76})$$

$$\frac{\partial \rho v}{\partial t} + v d_1 + \rho d_4 + \frac{\partial \rho v v}{\partial y} + \frac{\partial \rho v w}{\partial z} = \frac{\partial \tau_{2j}}{\partial x_j}, \quad (\text{A.77})$$

$$\frac{\partial \rho w}{\partial t} + w d_1 + \rho d_5 + \frac{\partial \rho w v}{\partial y} + \frac{\partial \rho w w}{\partial z} = \frac{\partial \tau_{3j}}{\partial x_j}, \quad (\text{A.78})$$

$$\frac{\partial \rho T}{\partial t} + d_2 + \frac{\partial \rho v T}{\partial y} + \frac{\partial \rho w T}{\partial z} + \frac{1}{\bar{c}_v} p \frac{\partial v}{\partial y} + \frac{1}{\bar{c}_v} p \frac{\partial w}{\partial z} = \frac{1}{\bar{c}_v} \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) + \dots, \quad (\text{A.79})$$

$$\frac{\partial Y_i}{\partial t} + d_{\text{SP},i} + v \frac{\partial \rho Y_i}{\partial y} + w \frac{\partial \rho Y_i}{\partial z} = - \frac{1}{\rho} \frac{\partial \rho Y_i V_{i,j}}{\partial x_j}. \quad (\text{A.80})$$

τ_{ij} corresponds to the viscous stress tensor and the subscripts 1, 2 and 3 denote x -, y - and z -directions respectively.

The difference between the governing equations A.17-A.20 and the NSCBC's governing equations(A.75-A.80) is that the derivative terms with respect to x are replaced by the d_i except for viscous term in the NSCBC equations. d_i is given by the following relations:

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$$d_1 = \frac{\partial \rho u}{\partial x} = \frac{1}{c^2} \left[\mathcal{L}_2 + \frac{1}{2} (\mathcal{L}_5 + \mathcal{L}_1) \right], \quad (\text{A.81})$$

$$\begin{aligned} d_2 &= \frac{\partial \rho u T}{\partial x} + \frac{1}{\bar{c}_v} p \frac{\partial u}{\partial x} \\ &= \frac{1}{R^0 \sum (Y_i/W_i)} \left[\frac{u}{2} \left(\frac{\mathcal{L}_5}{u+c} + \frac{\mathcal{L}_1}{u-c} \right) + \rho R^0 T \sum_{i=1}^N \frac{\mathcal{L}_{\text{SP}, i}}{W_i} \right] \\ &\quad + \frac{T}{2c} \left(\frac{\mathcal{L}_5}{u+c} - \frac{\mathcal{L}_1}{u-c} \right) + \frac{1}{2c} \frac{R^0 \sum (Y_i/W_i) T}{\bar{c}_v} \left(\frac{\mathcal{L}_5}{u+c} - \frac{\mathcal{L}_1}{u-c} \right), \end{aligned} \quad (\text{A.82})$$

$$d_3 = \frac{\partial u u}{\partial x} = \frac{1}{2\rho c} (\mathcal{L}_5 - \mathcal{L}_1), \quad (\text{A.83})$$

$$d_4 = \frac{\partial u v}{\partial x} = \mathcal{L}_3, \quad (\text{A.84})$$

$$d_5 = \frac{\partial u w}{\partial x} = \mathcal{L}_4, \quad (\text{A.85})$$

$$d_{\text{SP}, i} = u \frac{\partial Y_i}{\partial x} = \mathcal{L}_{\text{SP}, i}. \quad (\text{A.86})$$

Here, c corresponds to the speed of sound and computed as:

$$c = \sqrt{\frac{\gamma p}{\rho}}, \quad (\text{A.87})$$

and $\mathcal{L}_i$ denotes the the amplitude variations of the characteristic waves cross-

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ing the boundary. $\mathcal{L}_i$ is written as:

$$\mathcal{L}_1 = \lambda_1 \left(\frac{\partial p}{\partial x} - \rho c \frac{\partial u}{\partial x} \right), \quad (\text{A.88})$$

$$\mathcal{L}_2 = \lambda_2 \left(c^2 \frac{\partial \rho}{\partial x} - \frac{\partial p}{\partial x} \right), \quad (\text{A.89})$$

$$\mathcal{L}_3 = \lambda_3 \frac{\partial v}{\partial x}, \quad (\text{A.90})$$

$$\mathcal{L}_4 = \lambda_4 \frac{\partial w}{\partial x}, \quad (\text{A.91})$$

$$\mathcal{L}_5 = \lambda_5 \left(\frac{\partial p}{\partial x} + \rho c \frac{\partial u}{\partial x} \right), \quad (\text{A.92})$$

$$\mathcal{L}_{\text{SP}, i} = \lambda_{\text{SP}, i} \frac{\partial Y_i}{\partial x}. \quad (\text{A.93})$$

λ_i denotes the characteristic velocity of each characteristic wave, and given by:

$$\lambda_1 = u - c, \quad (\text{A.94})$$

$$\lambda_2 = \lambda_3 = \lambda_4 = \lambda_{\text{SP}, i} = u, \quad (\text{A.95})$$

$$\lambda_5 = u + c. \quad (\text{A.96})$$

Perfectly non-reflecting conditions

The amplitude variations of the waves entering into the computational domain $\mathcal{L}_i$ is set to zero to obtain the perfectly non-reflecting conditions.

$$\mathcal{L}_i = 0. \quad (\text{A.97})$$

The derivative terms that appear in $\mathcal{L}_i$ are calculated from the interior points. In addition to the equation above, the following condition is needed.

$$\frac{\partial \tau_{11}}{\partial x} = 0. \quad (\text{A.98})$$

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Non-reflecting conditions

In case of the perfectly non-reflecting conditions, the information of pressure at infinity is not fed back to the computational domain. Similar to the perfectly non-reflecting conditions, $\mathcal{L}_2$ $\mathcal{L}_{SP,i}$ are set to zero for the non-reflecting conditions as well.

$$\mathcal{L}_2 = \mathcal{L}_3 = \mathcal{L}_4 = \mathcal{L}_5 = \mathcal{L}_{SP,i} = 0. \quad (\text{A.99})$$

$\mathcal{L}_{1,NF}$ is used to denote the constant pressure at infinity instead of the $\mathcal{L}_1$ in the perfectly non-reflecting conditions, and it is defined as:

$$\mathcal{L}_{1,NF} = K (p - p_\infty). \quad (\text{A.100})$$

Here, p_∞ is the constant pressure at infinity, and K can be determined by:

$$K = \frac{\sigma (1 - M^2) c}{L_0}, \quad (\text{A.101})$$

where, σ is a constant, M is the maximum of Mach number in the flow and L_0 is the characteristic size of the domain. If $\sigma = 0$, the magnitude of reflected wave K becomes 0 and corresponds to the perfectly non-reflecting conditions. Additional conditions for the non-reflecting conditions are as follows:

$$\frac{\partial \tau_{12}}{\partial x} = 0, \quad (\text{A.102})$$

$$\frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) = 0, \quad (\text{A.103})$$

$$\frac{\partial}{\partial x} (\rho Y_i V_{i,x}) = 0. \quad (\text{A.104})$$

A.3.4 Time integration

A low storage third-order Runge-Kutta scheme [100] is used to integrate the governing equations in time. A variable u at an instance n (u^n) is advanced in time into u^{n+1} by three steps with a time stepping size Δt by:

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$$\Delta u^n = \left(\frac{\partial u_k}{\partial t} \right)^n, \quad (\text{A.105})$$

$$u^{n'} = u^n + \Delta u^n \times \frac{1}{3} \Delta t, \quad (\text{A.106})$$

$$\Delta u^{n'} = \left\{ -\frac{5}{9} \Delta u^n + \left(\frac{\partial u}{\partial t} \right)^{n'} \right\}, \quad (\text{A.107})$$

$$u^{n''} = u^{n'} + \Delta u^{n'} \times \frac{15}{16} \Delta t, \quad (\text{A.108})$$

$$\Delta u^{n''} = \left\{ -\frac{153}{128} \Delta u^{n'} + \left(\frac{\partial u}{\partial t} \right)^{n''} \right\}, \quad (\text{A.109})$$

$$u^{n+1} = u^{n''} + \Delta u^{n''} \times \frac{8}{15} \Delta t. \quad (\text{A.110})$$

This scheme is an explicit scheme that requires a time step size, Δt , smaller than the smallest time scale of the flow field to ensure numerical stability. In the DNS of reacting flows, Δt can be determined based on the Courant number, the chemical time scale, or other methods. The Courant–Friedrichs–Lewy (CFL) condition, which requires the time step to be less than a certain value to assure numerical stability, becomes more severe in case of reacting flows. This is because the speed of sound increases in the high-temperature regions due to combustion, which requires a smaller grid size for spatial resolution. When the smallest chemical time scale is much smaller than the Δt , even higher resolution is needed. However, integration in such a small time step size is not feasible due to high computational expense.

To alleviate the time step size restriction due to the small chemical time scales, the multi-time scale (MTS) method [101] is implemented for the chemical reaction terms in energy and species conservation equations. In addition to MTS, correlated adaptive chemistry and transport (CO-DACT) [69, 70] is used to reduce the computational cost even further by using reduced chemical mechanisms and reducing the computation of transport properties in the domain, wherever necessary. These methods are briefly explained as follows.

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Multi-time scale (MTS) method

The terms in the governing equations of the reacting flows, except for the chemical reaction term, are integrated in time, using a third-order Runge-Kutta scheme, as explained before. The intermediate time step of the temperature (T^*) and reactive species (Y_i^*) are calculated as:

$$\begin{aligned} \frac{\rho T^* - \rho T^n}{dt} = & -\nabla \cdot (\rho \mathbf{u} T) + \frac{1}{\bar{c}_v} \nabla \cdot (\lambda \nabla T) - \frac{1}{\bar{c}_v} \sum_{i=1}^{N_s} (\rho Y_i \mathbf{V}_i c_{p,i} \cdot \nabla T) \\ & - \frac{T}{\bar{c}_v} \sum_{i=1}^{N_s} [R_i \nabla \cdot (\rho Y_i \mathbf{V}_i)] - \frac{1}{\bar{c}_v} \mathbf{P} : (\nabla \mathbf{u}), \end{aligned} \quad (\text{A.111})$$

$$\frac{\rho Y_i^* - \rho Y_i^n}{dt} = \nabla \cdot (\rho \mathbf{u} Y_i) - \nabla \cdot (\rho Y_i \mathbf{V}_i). \quad (\text{A.112})$$

The multi-times scale (MTS) [101] method is used to advance the chemical reaction terms in time, such that T^{n+1} , Y_i^{n+1} are determined as the following.

$$\frac{\rho T^{n+1} - \rho T^*}{dt} = -\frac{1}{\bar{c}_v} \sum_{i=1}^N (h_i \omega_i) + \frac{T}{\bar{c}_v} \sum_{i=1}^N (R_i \omega_i), \quad (\text{A.113})$$

$$\frac{\rho Y_i^{n+1} - \rho Y_i^*}{dt} = \omega_i. \quad (\text{A.114})$$

MTS [101] is an algorithm that integrates ordinary differential equations (ODEs) associated with chemical reactions, using a large Δt . This method assigns each chemical species, Y_i , into one integration group with an index M based on its chemical time scale, τ_i . The index of the integration group (M) in which Y_i belongs to is obtained as

$$M = \log_{10}(\Delta t / \tau_i) + 1. \quad (\text{A.115})$$

Species in the M -th group are integrated using a time step Δt_M , which is given as :

$$\Delta t_M = \Delta t / 10^{(M-1)}. \quad (\text{A.116})$$

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The integration procedure starts with the smallest Δt_M . After the M -th group is converged, the species mass fractions in the M -th group are fixed, and the ODE system continues to be integrated using Δt_{M-1} . This method enables a large Δt to be used as a global time-stepping for DNS to integrate the chemical reaction term in time. In addition, this method decreases the computational expense as it allows the use of a timescale larger than the smallest chemical timescale.

Correlated adaptive chemistry and transport (CO-DACT)

The correlated adaptive chemistry (CO-DAC) method [69] constructs a phase space that consists of a few key parameters, such as temperature and mass fractions of fuel, oxidizer, and important radicals. Instantaneous phase parameters at a grid point are compared with another reference point, which differs in time and space, and the correlation of these two points in the phase space is then examined. The threshold values to determine the correlation can be specified by the user. If the phase parameters at these two points are correlated, then the reduced chemical mechanism used for the reference point is reused for the correlated grid point. If the phase parameters are not correlated with other reference points, path flux analysis (PFA) is used to generate a new reduced chemical mechanism [102].

Correlated adaptive chemistry and transport (CO-DACT) method [70] further decreases the computational cost by applying a reduction to the computation of the transport properties, such as viscosity, diffusivity, and thermal conductivity, in a similar way to the procedure applied in CO-DAC. The transport calculations are reduced by the phase parameters, which are temperature and molar fractions of the first several abundant species. Similar to the chemical mechanism in CO-DAC, CO-DACT correlates the transport properties at two points, and if the phase parameters at a grid point are correlated with another reference point, then the transport properties at that point are not calculated.

Appendix B

Detailed chemical kinetic mechanism of $\text{H}_2\text{-O}_2$ combustion

Table B.1: Reactive species considered for the chemical kinetic mechanism [71]

No.	Species
1	H_2
2	O_2
3	O
4	OH
5	H_2O
6	H
7	HO_2
8	H_2O_2
9	N_2

APPENDIX B. DETAILED CHEMICAL KINETIC MECHANISM OF
H₂-O₂ COMBUSTION

Table B.2: Detailed reaction mechanism [71]

			A	n	E
H ₂ /O ₂ chain reactions					
R1	H + O ₂ = O + OH		3.55×10^{15}	-0.41	16.6
R2	O + H ₂ = H + OH		5.08×10^4	2.67	6.29
R3	H ₂ + OH = H ₂ O + H		2.16×10^8	1.51	3.43
R4	O + H ₂ O = OH + OH		2.97×10^6	2.02	13.4
H ₂ /O ₂ dissociation/recombination reactions					
R5	H ₂ + M = H + H + M ^a		4.58×10^{19}	-1.40	104.38
	H ₂ + Ar = H + H + Ar		5.84×10^{18}	-1.10	104.38
	H ₂ + He = H + H + He		5.84×10^{18}	-1.10	104.38
R6	O + O + M = O ₂ + M ^a		6.16×10^{15}	-0.50	0.00
	O + O + Ar = O ₂ + Ar		1.89×10^{13}	0.00	-1.79
	O + O + He = O ₂ + He		1.89×10^{13}	0.00	-1.79
R7	O + H + M = OH + M ^a		4.71×10^{18}	-0.50	0.00
R8	H + OH + M = H ₂ O + M ^b		3.8×10^{22}	-2.00	0.00
Formation and consumption of HO ₂					
R9	H + O ₂ + M = HO ₂ + M ^c	k_0	6.37×10^{20}	-1.72	0.52
	H + O ₂ + M = HO ₂ + M ^d	k_0	9.04×10^{19}	-1.50	0.49
		k_∞	9.04×10^{19}	-1.50	0.49
R10	HO ₂ + H = H ₂ + O ₂		1.66×10^{13}	0.00	0.82
R11	HO ₂ + H = OH + OH		7.08×10^{13}	0.00	0.30
R12	HO ₂ + O = OH + O ₂		3.25×10^{13}	0.00	0.00
R13	HO ₂ + OH = H ₂ O + O ₂		2.89×10^{13}	0.00	-0.50
Formation and consumption of H ₂ O ₂					
R14	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂ ^e		4.20×10^{14}	0.00	11.98
	HO ₂ + HO ₂ = H ₂ O ₂ + O ₂		1.30×10^{11}	0.00	-1.63
R15	H ₂ O ₂ + M = OH + OH + M ^f	k_0	1.20×10^{17}	0.00	45.5
		k_∞	2.95×10^{14}	0.00	48.4
R16	H ₂ O ₂ + H = H ₂ O + OH		2.41×10^{13}	0.00	3.97
R17	H ₂ O ₂ + H = H ₂ + HO ₂		4.82×10^{13}	0.00	7.95
R18	H ₂ O ₂ + O = OH + HO ₂		9.55×10^6	2.00	3.97
R19	H ₂ O ₂ + OH = H ₂ O + HO ₂ ^e		1.00×10^{12}	0.00	0.00
	H ₂ O ₂ + OH = H ₂ O + HO ₂		5.80×10^{14}	0.00	9.56

In Table B.2, units are $\text{cm}^3\text{-mol-s-kcal-K}$, and $k = AT^n \exp(-E/RT)$. Corresponding footnotes are as follows [71].

^a Efficiency factors are: $\varepsilon_{\text{H}_2\text{O}} = 12.0$, $\varepsilon_{\text{H}_2} = 2.5$, $\varepsilon_{\text{Ar}} = 0.75$, and $\varepsilon_{\text{He}} = 0.75$

^b Efficiency factors are: $\varepsilon_{\text{H}_2\text{O}} = 12.0$, $\varepsilon_{\text{H}_2} = 2.5$, $\varepsilon_{\text{Ar}} = 0.38$, and $\varepsilon_{\text{He}} = 0.38$

^c When the main bath gas is N_2 ($M=\text{N}_2$). Troe parameter is $F_c = 0.8$. Efficiency factors are: $\varepsilon_{\text{H}_2\text{O}} = 11.0$, $\varepsilon_{\text{H}_2} = 2.0$, and $\varepsilon_{\text{O}_2} = 0.78$.

^d When the main bath gas is Ar or He ($M=\text{Ar}$ or He). Troe parameter is $F_c = 0.5$. Efficiency factors are: $\varepsilon_{\text{H}_2\text{O}} = 16.0$, $\varepsilon_{\text{H}_2} = 3.0$, $\varepsilon_{\text{O}_2} = 1.1$, and $\varepsilon_{\text{He}} = 1.2$.

^e R14 and R19 are expressed as the sum of two rate expressions.

^f Troe parameter is $F_c = 0.5$. Efficiency factors are: $\varepsilon_{\text{H}_2\text{O}} = 12.0$, $\varepsilon_{\text{H}_2} = 2.5$, $\varepsilon_{\text{Ar}} = 0.64$, and $\varepsilon_{\text{He}} = 0.64$.

Acknowledgements

I would like to start by expressing my appreciation and gratitude to my academic supervisor, Prof. Tanahashi, for allowing me to have precious experience in this lab and his continuous support throughout my research. I would also like to thank Assoc. Prof. Shimura for his supports. I am sincerely grateful to Assist. Prof. Minamoto, who guided and encouraged me patiently.

I would also like to thank our secretary, Ms. Kawamura, for her practical support and constant kindness. I am grateful to the past and present members of the Reactive Gas Dynamics Lab, starting with Dr. Osawa, who constantly guided and supported me, even when he was thousands of kilometers away. All the conversations we had are terribly missed. I would like to thank Dr. Park for introducing me to TTX and helping me with the chemistry-related parts of combustion. I am also grateful to Mohamed, who introduced me to the non-premixed flames. I should also thank Son, Kumar, and Fuse for their friendship outside the lab. I had a pleasant time at the conferences, thanks to Nakagama, Nakazawa, Atagi, and Sasaki. I am also grateful to Wang, Hisakado, Yokoyama, Nakagome, Sakai, Lu, Hattori, Urasaki, Sato and Huang. Finally, special thanks to Kherlen for his friendship and support.

My life as a Ph.D. candidate in Japan was a fantastic experience with all its ups and downs. First, I want to thank Erdem for planting the idea of coming here, helping me adjust, and introducing me to two amazing people: Gülin and Ash, whose discussions helped me maintain my “human side”. I would also like to thank Rami for his random cheer up messages. The second

half of my life in Japan was shadowed by the pandemic. However, I had the best friends to survive this most peculiar period of my life: Haris and Giedre. I do not have enough words to describe how much they mean to me. I would also like to thank my “sistas”, and all the other friends in Turkey and the US, who cheered for me and made me realize friendship knows no distance. Last but not least, I am deeply grateful to my family, who supported me unconditionally. Their love and trust gave me the strength to continue.

The financial support of the Ministry of Education, Culture, Sports, Science and Technology, Japan (MEXT) during my stay is also acknowledged.