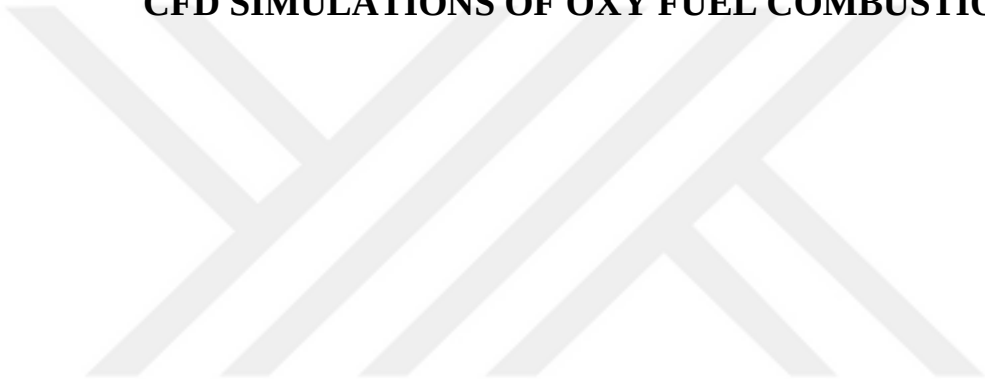


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GRADUATE SCHOOL OF NATURAL AND APPLIED SCIENCES

CFD SIMULATIONS OF OXY FUEL COMBUSTION



AYKUT YILDIRIM
A THESIS SUBMITTED FOR THE DEGREE OF
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DEPARTMENT OF MECHANICAL ENGINEERING

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**THESIS SUPERVISOR
ASSIST.PROF. DR. SALİH ÖZEN ÜNVERDİ**

**GEBZE
2022**

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SUMMARY

In this thesis, Oxy-Fuel flames are analyzed by Reynolds Avaraged Navier Stokes simulations. Non-premixed Oxy-Fuel flames are simulated in coaxial cylindrical burner configuration. Fuel mixture comprised of 25% methane (CH_4) and 75% oxidizer by volume is fed into the reactor. Volume fractions of 25%, 30% and 35% O_2 are considered in the oxidizer stream wich is a mixture of O_2 and CO_2 . A pilot flow which is a mixture of CH_4 , O_2 and CO_2 with 77% fuel to oxidizer ratio is fed into reactor from the annular gap surrounding the central fuel nozzle. In addition, an oxidizer stream surrounding the fuel and pilot streams is fed into reactor as a coflow. Furthermore, the effect of reactant temperature on flame characteristics is analyzed by simulating oxy-fuel flames with various reactant temperatures of 300 K, 500 K, 700 K. CFD simulations are performed by a featured combustion model in the literature. Steady Laminar Flamelet Model decouples combustion chemistry from Reynolds Avaraged Navier Stokes (RANS) equations. In addition to RANS equations two more equations are solved for mean mixture fraction and its variance. Decoupled chemistry is tabulated as a look-up table in mixture fraction space for different scalar dissipation rates. By applying β -PDF integration, enthalpies and species mass fraction data could be looked-up by RANS equations. Transport and thermal properties change according to oxidizer composition and the temperature of the reactants. Following results are obtained from the CFD simulations: Increasing O_2 volume ratio of the oxidizer extends the flammability limits. For a 25% O_2 content of the oxidizer stream, reaction resistance against aerodynamic strain is weak. Flame could be anchored to the injector if volume fraction of O_2 in oxidizer stream is 35%. Flame temperature increases and flammability limits are extended by increasing the reactor inlet temperature of the reactants. Flame length decreases as temperature of the reactants is increased.

Key Words: Oxy-Fuel combustion, Reynolds-Averaged Navier-Stokes Equations, Flamelet Model, CO_2 dilution.

ÖZET

Bu çalışmada oksî-yakıt alevleri Reynolds-Ortalama Navier-Stokes Denklemleri ile incelenmiştir. Ön karışimsız oksî-yakıt alev simülasyonları eş eksenli silindirik enjektör konfigürasyonunda gerçekleştirilmiştir. Hacimsel olarak %25 metan (CH_4) %75 yakıcıdan oluşan yakıt karışımı reaktöre beslenmiştir. Yakıcı olarak %25, %30, %35 O_2 hacim oranlarına sahip O_2+CO_2 karışımları göz önüne alınmıştır. %77 yakıt/yakıcı oranında metan (CH_4) + yakıcı (O_2+CO_2) karışımı olan pilot akım merkezi yakıt menfezini çevreleyen aralıktan reaktöre beslenmiştir. Ayrıca, yakıt ve pilot akımlarını çevreleyen bir yakıcı akımı eş-akış olarak reaktöre beslenmiştir. Ek olarak, reaksiyona giren karışımların sıcaklığının alev karakteristikleri üzerindeki etkisi çeşitli tepken giriş sıcaklıkları için (300 K, 500 K, 700 K) oksî-yakıt alev benzeşimleri gerçekleştirilerek incelenmiştir. CFD simülasyonları literatürde öne çıkan bir yanma modeli ile gerçekleştirilmiştir. Sabit Rejim Laminer Alevcik Modeli yanma kimyasını Reynolds ortalama Navier-Stokes (RANS) denklemlerinden ayırır. Reynolds ortalama Navier Stokes denklemlerine ek olarak ortalama karışım oranı ve varyansı için iki denklem daha çözülür. Ayırıştırılan kimya, referans bir tablo olarak kullanılmak üzere çeşitli skaler dağılma hızları için karışım oranı uzayında tablolastırılmıştır. β -PDF intgrasyonu uygulayarak entalpi ve kimyasal bileşiklerin kütle oranı verileri RANS denklemleri tarafından referans tablo olarak kullanılabilir hale getirilmiştir. Transport ve ısı özellikler, yakıcı kompozisyonu ve tepkenlerin giriş sıcaklığına bağlı olarak değişir. CFD benzeşimleriyle aşağıdaki sonuçlar bulunmuştur: Yakıcı içinde O_2 hacimsel oranının arttırılması yakılabilirlik limitlerini genişletir. Yakıcıda %25 oranında O_2 kullanıldığında aerodinamik uzamaya karşı reaksiyon direnci zayıftır. Yakıcı akımda O_2 hacim oranı %35 olduğunda alev enjektöre sabitlenebilmiştir. Tepkenlerin reaktöre giriş sıcaklığı arttıkça alev sıcaklığı artar ve yakılabilirlik limitleri genişler. Artan tepken giriş sıcaklığı ile alev boyu kısalmır.

Anahtar Kelimeler: Oksî-Yakıt Yanması, Reynolds-Ortalama Navier-Stokes Denklemleri (RANS), Alevcik Modeli, CO_2 seyreltmesi.

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LIST OF ABBREVIATIONS AND ACRONYMS

<u>Abbreviations</u> <u>and Acronyms</u>	<u>Explanations</u>
∇	: Nabla operator
ρ	: Density
μ	: Dynamic viscosity
ε	: Turbulent dissipation rate
μ_t	: Turbulent viscosity
$\tilde{\sigma}$	: Shear stress tensor
k	: Turbulent kinetic energy
h	: Entalphy
T	: Temperature
Y_k	: Species mass fraction
c_p	: Heat capacity at constant pressure
χ	: Scalar dissipation rate
χ_{st}	: Scalar dissipation rate at stoichiometry
$\vec{\delta}$	: Kronecker delta
t	: Time
D	: Diffusion coefficient
K	: Kelvin
Le	: Lewis number
Da	: Damkohler number
Re	: Reynold number
Z	: Mixture fraction
Φ	: Equivalence ratio
O ₂	: Oxygen
OH	: Hydroxide
CO	: Carbon monoxide
CO ₂	: Carbon Dioxide
CH ₄	: Methane
RANS	: Reynolds Averaged Navier Stokes

CFD	:	Computational Fluid Dynamics
SLFM	:	Steady Laminar Flamelet Model
FPV	:	Flamelet Progress Variable
LES	:	Large Eddy Simulations
DNS	:	Direct Numerical Simulation
CMC	:	Conditional Moment Clousure
PDF	:	Probability Density Function



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1. INTRODUCTION

Turbulent combustion is a complex phenomenon in which turbulent flow and chemical reactions take place and interact with each other. Turbulent combustion is classified as premixed and non-premixed. In premixed combustion fuel and oxidizer streams are mixed before they are fed into a combustion chamber. However, in non-premixed combustion fuel and oxidizer streams separately enter the combustion chamber. In this thesis non-premixed combustion is considered.

In industry non-premixed combustion is preferred in a wide range of applications because of design amenities and being safe to operate compared to premixed combustion. In combustion modelling, turbulent flow physics and chemical kinetics should be considered to predict flame characteristics. Computational Fluid Dynamics (CFD) is a featured method to analyze behaviour of flames and design efficient combustors.

There are three main strategies in numerical simulations of combustion by Computational Fluid Dynamics. These are Reynolds-Averaged Navier-Stokes Simulations (RANS), Large Eddy Simulations (LES) and Direct Numerical Simulations (DNS). In RANS context all eddy motions are modelled. However, in LES eddies larger than the grid scale are resolved while subgrid scale eddies are modeled. In DNS context, all eddy motions from large scale to Kolmogorov viscous scale are resolved. Although DNS and LES are capable of accurately capturing turbulent flow physics, these methods are computationally expensive due to their grid resolution requirements and time dependent nature of flow simulations. Therefore, in this study combustion physics is modeled under RANS framework.

1.1. Goals and Motivation

Among various emissions reduction methods available today, carbon capture technologies are utilized to eliminate release of CO_2 to the atmosphere. Oxy-fuel combustion is a carbon capture technology which avoids or significantly lowers NO_x emissions and decreases flue gas volume considerably due to the lack of N_2 in the oxidizer. In oxy-fuel combustion, either pure or diluted O_2 is utilized as the oxidizer instead of air. In this thesis, characteristics, and emissions of piloted nonpremixed

flames formed by oxy-fuel combustion of CH_4 with O_2 which is diluted with CO_2 are studied by CFD simulations. Our primary objective is to determine the effects of dilution of O_2 with CO_2 and the inlet temperature of the reactants on piloted flame characteristics and emissions.

Combustion process is a complicated phenomenon in which continuity, momentum, energy, and species transport equations are coupled to chemical kinetics. Steady Laminar Flamelet Model is a time-efficient method to simulate combustion environment. Steady Laminar Flamelet Model which assumes chemical time scale is significantly smaller than turbulent time scale, solves chemical kinetics equations separately from transport equations [Peters, 1984]. A look-up table of tabulated mean sensible enthalpy and mean species mass fractions according to mean mixture fraction, mean stoichiometric mixture scalar dissipation rate and mixture fraction variance, which are provided by the turbulent CFD code, are utilized in the solution of the Reynolds averaged continuity, momentum, energy, mixture fraction and mixture fraction variance transport equations by CFD.

In this study, SLFM model is utilized to simulate the effect of CO_2 dilution ratio and inlet temperature of the reactants on flame characteristics and emissions under RANS framework with full chemical reaction mechanism GRI 3.0. The thesis is a contribution to the literature because the effects of CO_2 dilution and oxidizer temperature on flame characteristics and emissions of non-premixed oxy-fuel combustion of CH_4 have not been studied by SLFM so far.

2. BACKGROUND AND LITERATURE REVIEW

Oxy-fuel combustion is one of the carbon capture technologies which aims to reduce CO emissions [Zheng, 2011]. In oxy-fuel combustion fuel is oxidized directly by O_2 instead of air. Lack of N_2 leads to excessively increased flame temperatures. Instead of air, O_2 diluted with CO_2 is utilized as the oxidizer to control the flame temperature and the CO_2 content of the flue gases is captured by condensation and fed back into the reactor [Buhre et al., 2005]. As compared to air fired combustion, flame temperature and residence time against strain rate have different characteristics as pointed out in various articles [Chen et al., 2007] [Li et al., 2016] [Maruta et al., 2007] [Habisreuther et al., 2019].

Many studies have been conducted to investigate oxy-fuel flames [Xie et al., 2013] [Ditaranto and Hals, 2006] [Saanum and Ditaranto, 2017] [Habib et al., 2017] [Han et al., 2015] [Shakeel et al., 2018]. CO_2 dilution ratio is an important parameter in determining border of extinction and flammability characteristics of the flame. CO_2 dilution of combustion has been investigated in the literature based on chemical effects [Zhang et al., 1992] [Glarborg and Bentzen, 2008] [Masri and Barlow, 2006] [Dobó et al., 2019] [Sabia et al., 2015] [T. H. Kim et al., 2016]. Also temperature of the reactants effects flame characteristics based on flammability, extinction limits and mixing behaviour [Oh and Hong, 2016] [Jana et al., 2020] [Seepana and Jayanti, 2016]. O_2/CO_2 ratio and temperature of the reactants change mixture transport properties, density, heat capacity and flame temperature [Rashwan, 2018]. So, feeding temperature of the reactants and CO_2 dilution ratio are important parameters in investigating these differences.

Combustion modelling is a complex issue in which detailed chemical mechanism and its coupling with turbulence physics should be considered. In turbulent physics, turbulent kinetic energy generation and dissipation occur at different length scales. In CFD simulations these length scales can be either modelled or resolved. Resolved physics of turbulence give insight into the detailed behaviour of the flow structure. However, modelling of turbulent scales give insight into mean values and tendency of the flow field. In RANS turbulent length scales are modeled. In RANS simulations although turbulent physics can not be resolved accurately, mean scalar and

vector fields can be predicted effectively. A variety of RANS models exist in the literature [Sayyed et al., 2007] [Pope, 1985] [Veynante and Vervisch, 2002] [Wegner et al., 2004].

Several models such as Probability Density Function (PDF) transport models [Pope, 1985], Conditional Moment Clousure (CMC) model [Bilger, 1992], Laminar Flamelet Models [Peters, 1984] have been developed to study non-premixed combustion. A. Garmory have simulated oxy-fuel flames by Conditional Moment Clousure [Garmory & Mastorakos, 2015]. Moreover, Flamelet approach is a featured method to account for finite rate chemistry. In this concept reaction time scales are assumed to be much smaller than turbulence time scales. Therefore, chemical kinetics calculations can be decoupled from CFD simulations which decreases the computing time significantly. Laminar flamelet concept can be divided into two categories: Steady/Unsteady Laminar Flamelet Models (SLFM/ULFM) and Flamelet Progress Variable Models [Pierce & Moin, 2001]. FPV model is an extended version of SLFM which utilizes reaction progress variable. Mahmoud Rihab has studied oxy-fuel combustion by FPV method [Mahmoud et al., 2018]. Compared to SLFM, FPV is a better approach in predicting unsteady flame phenomena such as re-ignition and local extinction. Furthermore, Steady Laminar Flamelet method has been evaluated in oxy-fuel framework by Rene Prieler [Prieler et al., 2014].

In this study, Steady Laminar Flamelet approach coupled with Reynold-Avaraged Navier-Stokes (RANS) equations is applied to simulate oxy-fuel combustion of CH_4 for various O_2/CO_2 ratios of the oxidizer stream and temperatures of the reactants. Simulations are performed by flameletFoam [Müller et al., 2013] which is developed under OpenFOAM. This solver has akready been utilized in simulations of oxy-fuel flames at different pressures by Mingjie Xiong [Xiong et al., 2020]. Also flameletFoam has been validated by simulations of Sandia D flame [Barlow and Frank, 2007] in the study of Hagen Muller [Müller et al., 2013]. In section 3.1, Steady Flamelet Model (SLFM) is introduced.

2.1. Sandia D Piloted CH_4 /Air Jet Flame

Experimental data of the flame temperature and mass fractions of major species of the Sandia D piloted diffusion flame recorded by Sandia National Laboratories

[Barlow and Frank, 2007] is widely utilized in validation of CFD codes [Di Renzo et al., 2015] [Pitsch and Steiner, 2000] [Ferraris and Wen, 2008].

In Sandia D piloted diffusion flame, a coaxial injector where the fuel and surrounding pilot streams are fed into a combustion chamber through a 7.2 mm diameter central nozzle and through the annular gap between the central nozzle and an 18.2 mm diameter outer nozzle is utilized. A co-flowing oxidizer stream surrounds both the fuel and pilot streams. Injector wall thicknesses between the fuel and pilot streams and between the pilot and co-flowing oxidizer streams are 0.25 mm. and 0.35 mm, respectively. Experiments are performed in a 30x30 cm rectangular co-flow wind tunnel.

2.2. Oxy-Fuel Piloted $\text{CH}_4/(\text{O}_2+\text{CO}_2)$ Jet Flame

In the oxy-fuel simulations conducted in this thesis, the composition of the gas mixture formed by the fuel, pilot and oxidizer streams is the same as that of the Sandia D flame reactants. However, instead of air, CO_2 diluted O_2 is used as oxidizer with various O_2/CO_2 ratios, i.e 25%, 30% and 35%. Furthermore, different reactant stream temperatures are considered. For 30% O_2/CO_2 ratio case, oxy-fuel flames formed by reactants with inlet temperatures of 300K, 500K and 700K are simulated. Mixture compositions are listed in Table 1. Also, Burner geometry and boundary conditions are assumed to be the same as those of the Sandia D piloted diffusion flame.

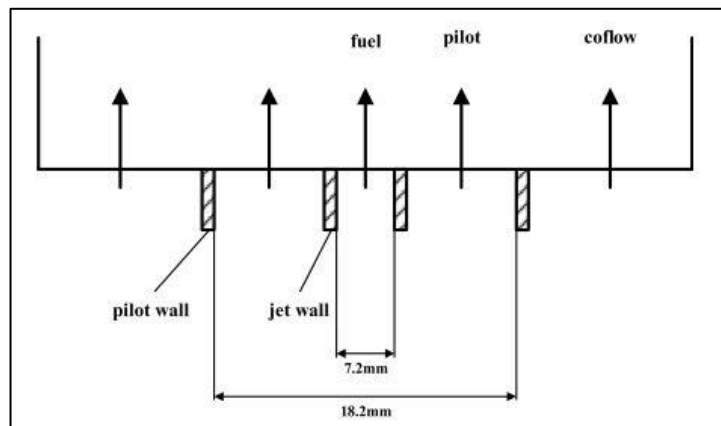


Figure 2. 1: Injector configuration and geometric dimensions.

3. THEORY AND GOVERNING EQUATIONS

Coupling of turbulence physics and reaction chemistry is modelled in CFD. However different length and time scales occur in this process. In this section solution of these issues within the context of RANS simulations with SLFM formulations is explained.

3.1. Reynolds Averaged Navier Stokes (RANS)

Reynolds-averaged Navier-Stokes equations can be derived in two steps. Firstly, dependent variables are decomposed into mean and fluctuation components by Reynolds decomposition given below:

$$f = \bar{f} + f'' \quad (3.1)$$

Secondly, density weighted averaging namely Favre averaging is applied. Favre averaging accounts for density variations in combustion problems. Favre averaging is expressed as

$$\tilde{f} = \frac{\overline{\rho f}}{\bar{\rho}} \quad (3.2)$$

After these manipulations are applied, some terms become zero and un-closed terms arise in the equation set. Favre-averaged conservation of mass and momentum equations can be written as

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_j}{\partial x_j} = 0 \quad (3.3)$$

$$\frac{\partial \bar{\rho} \tilde{U}}{\partial t} + \frac{\partial \bar{\rho} \tilde{U}_i \tilde{U}_j}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial \tilde{\sigma}}{\partial x_j} - \frac{\partial \bar{\rho} U'' U''}{\partial x_j} + \bar{\rho} \tilde{g} \quad (3.4)$$

where “ $\tilde{}$ ” denotes a Favre averaged quantity, while “ $\bar{}$ ” represents a time averaged mean quantity. $\tilde{\sigma}$ represents Favre-averaged shear stress tensor in equation (3.4).

Reynolds stress term $\bar{\rho}U''U''$ appearing in the momentum equations can be closed by k- ϵ turbulence model as

$$\bar{\rho}U''U'' = -2\mu_t\tilde{\gamma} - \frac{2}{3}\left(\mu_t\nabla\cdot\tilde{\vec{U}}\right)\vec{\delta} + \frac{2}{3}(\bar{\rho}\tilde{k}\vec{\delta}) \quad (3.5)$$

where, $\tilde{\gamma}$ represents Favre weighted strain rate, $\tilde{k}$ denotes the Favre weighted turbulent kinetic energy and $\vec{\delta}$ is the Kronocker delta. The kinetic energy and turbulent viscosity are defined as

$$\tilde{k} = \frac{1}{2}U''U'' \quad (3.6)$$

$$\mu_t = C_\mu\bar{\rho}\frac{\tilde{k}^2}{\tilde{\epsilon}} \quad (3.7)$$

where, C_μ is a constant equal to 0.09. $\tilde{k}$ and $\tilde{\epsilon}$ transport equations can be expressed as

$$\frac{\partial\bar{\rho}\tilde{k}}{\partial t} + \frac{\partial\bar{\rho}\tilde{U}\tilde{k}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\nabla\tilde{k}\right] + \tilde{G}_k - \bar{\rho}\tilde{\epsilon} \quad (3.8)$$

$$\frac{\partial\bar{\rho}\tilde{\epsilon}}{\partial t} + \frac{\partial\bar{\rho}\tilde{U}\tilde{\epsilon}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon}\right)\frac{\partial\tilde{\epsilon}}{\partial x_j}\right] + \left(C_{\epsilon 1}\frac{\tilde{\epsilon}G_k}{\tilde{k}}\right) - \left(C_{\epsilon 2}\bar{\rho}\frac{\tilde{\epsilon}^2}{\tilde{k}}\right) \quad (3.9)$$

Constants of this equation set are given as [Launder and Sharma, 1974]

$$\sigma_k = 1, \sigma_\epsilon = 1.3, C_{\epsilon 1} = 1.44, C_{\epsilon 2} = 1.92 \quad (3.10)$$

$$G_k = 2\mu_t\tilde{\delta}_{ij}\tilde{\delta}_{ij} : \text{turbulent kinetik energy production}$$

($\tilde{\delta}_{ij}$ is strain rate tensor)

3.2. Steady Laminar Flamelet Model

Steady Laminar Flamelet Model assumes turbulent flame is an ensemble of laminar flamelets. This assumption is valid under high Damkohler number regime conditions in which turbulent time scale is much bigger than chemical time scale. This method accounts for finiti-rate chemistry effects by considering detailed chemical mechanisms. However, SLFM is not good at capturing unsteady combustion physics such as flame extinction and re-ignition phenomena. Despite the pointed-out drawbacks, SLFM model can predict main flame charcteritics accurately.

In this method laminar flamelet calculations are decoupled from turbulent flow calculations which speeds up CFD calculations considerably. Flamelets are calculated by a 1-D counterflow diffusion flame solver. Enthalpy and species mass fractions are tabulated in mixture fraction domain for different scalar dissipation rates. Mixture fraction Z is a ratio of fuel amount in given mixture. At fuel inlet mixture fraction Z is unity, while at oxidizer inlet mixture fraction Z is zero. In mixture fraction space equations for species mass fractions and for temperature under $Le = 1$ assumption can be written as

$$\rho \frac{\partial Y_k}{\partial t} - \frac{1}{2} \rho \chi \frac{\partial^2 Y_k}{\partial Z^2} - \dot{w}_k = 0 \quad (3.11)$$

$$\rho \frac{\partial T}{\partial t} - \frac{1}{2} \rho \chi \left(\frac{\partial^2 T}{\partial Z^2} + \frac{1}{c_p} \frac{\partial c_p}{\partial Z} \frac{\partial T}{\partial Z} \right) + \frac{1}{c_p} \sum_{k=1}^n h_k \dot{w}_k = 0 \quad (3.12)$$

where, Y_k , h_k and $\dot{w}_k$ refer to k_{th} chemical species mass fraction, specific enthalpy and chemical source term provided by GRI 3.0 mechanism, respectively, T is the temperature, ρ is the density, c_p is the specific heat at constant pressure, and χ is the scalar dissipation rate which is defined as

$$\chi = 2D \left(\frac{\partial Z}{\partial y} \right)^2 \quad (3.13)$$

Scalar dissipation rate χ is a function of mixture fraction Z and time. However, its value for the stoichiometric mixture χ_{st} can be used instead. This parametrization is given in (J. S. Kim and Williams, 1997). χ_{st} represents strain effect against reaction

rate. When χ_{st} increases flame becomes extinct due to aerodynamic strain effect. In this thesis, 1-D counterflow diffusion flame calculations are conducted on Cantera software. Flamelets are tabulated for different strain rates by increasing the mass flow rate until extinction limits are reached. These flamelet tabulations store species mass fractions and temperature as functions of mixture fraction and scalar dissipation rate at stoichiometry ($Y_k(Z, \chi_{st})$ and $T(Z, \chi_{st})$).

3.2.1. Favre Presumed Probability Density Function

Favre presumed probability density function is utilized in calculating mean values of species mass fractions and temperature as follows:

$$\tilde{Y}_k = \int_0^\infty \int_0^1 Y_k(Z, \chi_{st}) P(Z, \chi_{st}) dZ d\chi_{st} \quad (3.14)$$

$$\tilde{T} = \int_0^\infty \int_0^1 T(Z, \chi_{st}) P(Z, \chi_{st}) dZ d\chi_{st} \quad (3.15)$$

Joint PDF is defined based on statistical independence as shown below

$$P(Z, \chi_{st}) = P(Z)P(\chi_{st})$$

PDF of scalar dissipation rate is $P(\chi_{st}) = \delta(\chi_{st} - \tilde{\chi}_{st})$. PDF of mixture fraction is assumed to be presumed β -PDF.

$$P(Z) = Z^{\alpha-1} (1-Z)^{\beta-1} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \quad (3.16)$$

where, Γ is the gamma function, and α and β are the parameters of β -PDF which are functions of mean mixture fraction $\tilde{Z}$ and mixture fraction variance $\tilde{Z}''^2$.

$$\alpha = \tilde{Z} \left(\frac{\tilde{Z}(1-\tilde{Z})}{\tilde{Z}''^2} - 1 \right) \quad (3.17)$$

$$\beta = (1-\tilde{Z}) \left(\frac{\tilde{Z}(1-\tilde{Z})}{\tilde{Z}''^2} - 1 \right) \quad (3.18)$$

CFD calculations in OpenFOAM depend on sensible enthalpy h_s . Therefore, temperature and thermodynamic data is converted to enthalpy by canteraToFoam utility. After this conversion and PDF integration, mean values of species mass fractions $\tilde{Y}_k$ and enthalpy $\tilde{h}_s$ are tabulated by means of mean values of mixture fraction $\tilde{Z}$, its variance $\tilde{Z}''^2$ and scalar dissipation rate at stoichiometric condition $\tilde{\chi}_{st}$. Tabulated chemistry is used as a look-up table by RANS equations. Apart from already pointed out RANS equations, two additional transport equations for mean mixture fraction $\tilde{Z}$ and its variance $\tilde{Z}''^2$ must be solved to close the equation set.

$$\frac{\partial \rho \tilde{Z}}{\partial t} + \frac{\partial \rho \tilde{U}_i \tilde{Z}}{\partial x_j} = \frac{\partial}{\partial x_j} \left((\mu_t + \mu) \frac{\partial \tilde{Z}}{\partial x_j} \right) \quad (3.19)$$

$$\frac{\partial \rho \tilde{Z}''^2}{\partial t} + \frac{\partial \rho \tilde{U}_i \tilde{Z}''^2}{\partial x_j} = \frac{\partial}{\partial x_j} \left((\mu_t + \mu) \frac{\partial \tilde{Z}''^2}{\partial x_j} \right) + 2(\mu_t + \mu) \left(\frac{\partial \tilde{Z}}{\partial x_j} \right)^2 - \rho \tilde{\chi} \quad (3.20)$$

Scalar dissipation rate is modeled as

$$\tilde{\chi} = C_\chi \frac{\epsilon}{k} \tilde{Z}''^2 \quad (3.21)$$

where, k and ϵ represents turbulent kinetic energy and its dissipation rate, respectively. C_χ is assumed to be 2.0 as seen in [Janicka and Peters, 1982].

4. SIMULATION DETAILS

In this thesis, SLFM coupled with RANS equations are solved to simulate Oxy-fuel diffusion flames of CH_4 and O_2 which is diluted with CO_2 . Solver which was developed in OpenFOAM environment by Hagen Muller is called flameletFoam [Müller et al., 2013]. The solver has already been validated by Sandia D flame data in Muller's paper. Experimental data of Sandia D flame can be found in article [Barlow & Frank, 2007]. In this thesis validation is checked by re-simulating the Sandia D flame.

In validation study Oxy-Fuel flame simulations are performed under the same configurations and conditions of the Sandia D flame. Sandia D flame injector configurations and boundary conditions can be seen in the paper of Barlow. However, in oxy-fuel simulations, O_2+CO_2 mixtures with a variety of compositions are utilized as oxidizer instead of air, which is the oxidizer of the Sandia D flame. In the CFD simulations performed in this thesis O_2 volume fractions of 25%, 30%, and 35% are considered in the oxidizer stream (O_2+CO_2 mixture). Furthermore, effects of the temperature of the reactants on flame characteristics are studied by considering three different inlet temperatures 300 K, 500K, and 700K for the case of O_2 volume fraction of 30% in the oxidizer.

4.1. Sandia D Flame Simulation

In this thesis, first, CFD code named flameletFoam is validated by Sandia D flame simulations. Although the CFD solver has already been validated by Sandia D flame data in a recent paper [Müller et al., 2013], accuracy and reliability of flameletFoam is reconfirmed by simulations performed within the scope of this thesis. Details of injector geometric dimensions, boundary conditions and experimental data of Sandia D flame can be found in the literature [Barlow and Frank, 2007].

Equations are solved on a 600x150 mm rectangular domain. Axisymmetric mesh which has 180000 cells is generated by forming 900 and 200 partitions in axial and radial directions, respectively. Mesh is plotted in the following figure.

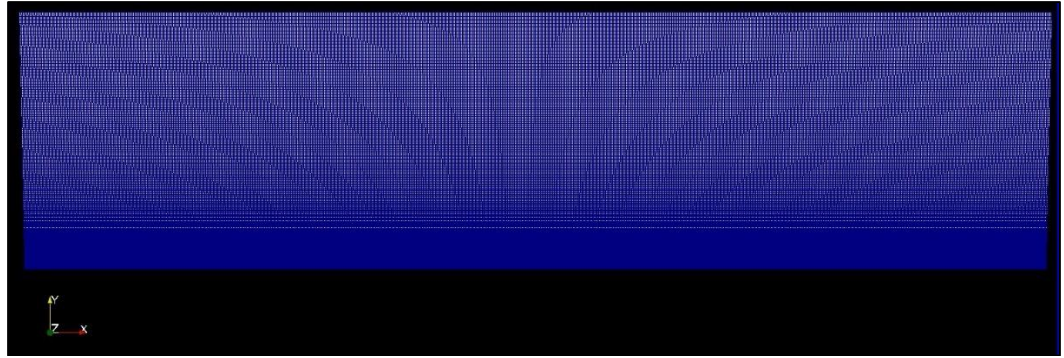


Figure 4. 1. Mesh with 180000 cells for axy-symmetric Sandia D flame simulations.

Axial temperature and mixture fraction distributions obtained by the simulations agreed well with the experimental data as shown in the following plots.

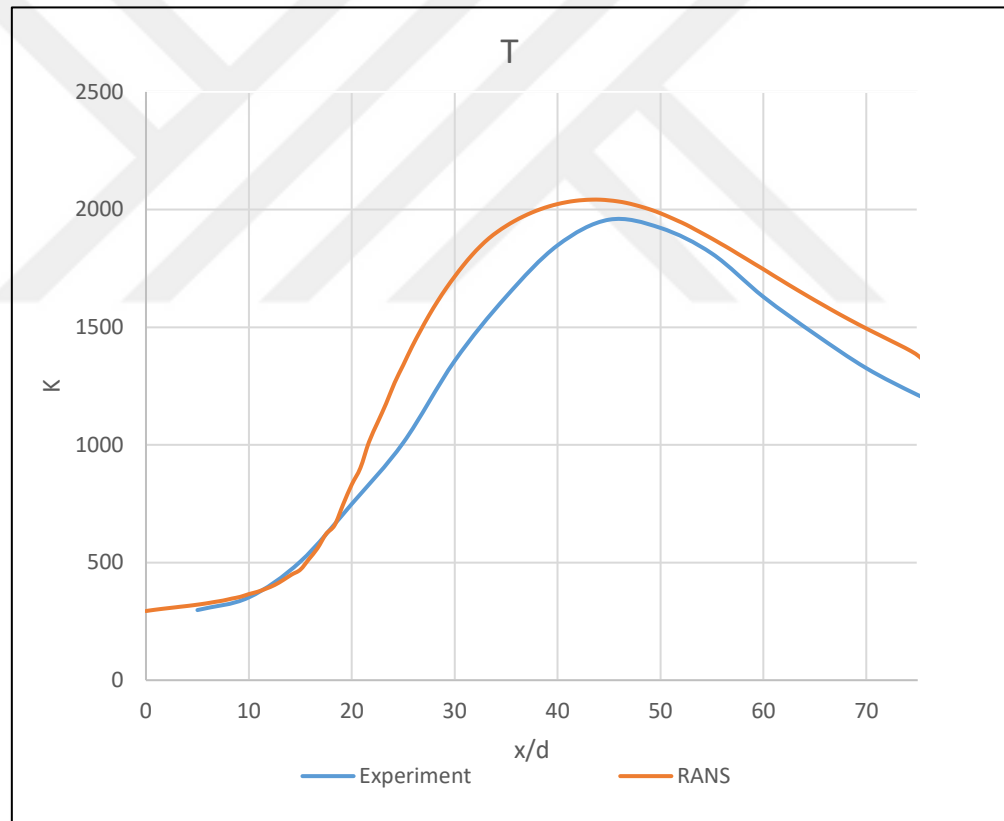


Figure 4. 2. Axial temperature distribution of the Sandia D flame.

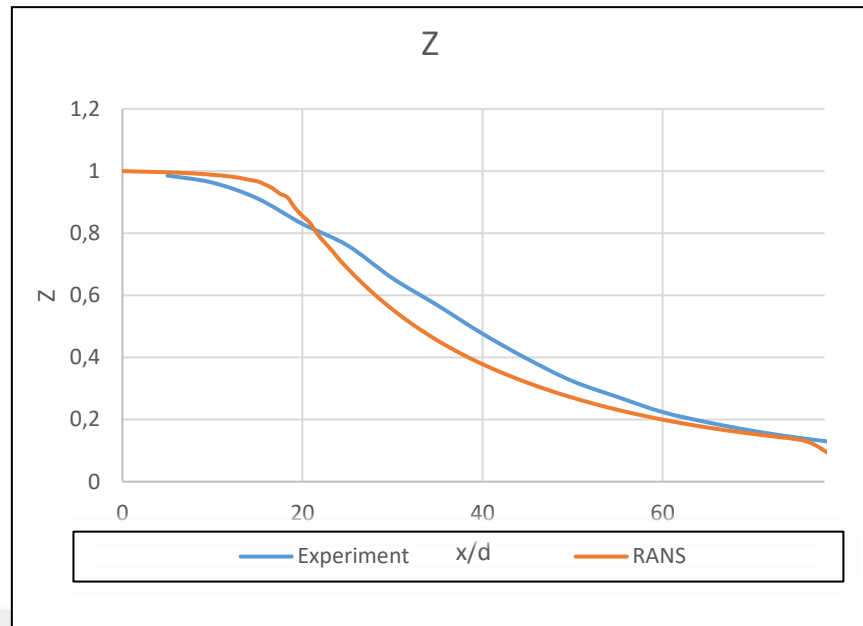


Figure 4.3. Axial mixture fraction distribution of the Sandia D flame.

However, far field radial temperature distributions of Sandia D flame are overpredicted by RANS results. Comparison of calculated and experimental radial temperature distributions at various axial locations are presented in the following figures. Overprediction of far field radial temperature profiles can be attributed to the lack of radiation modelling in the flameletFoam code.

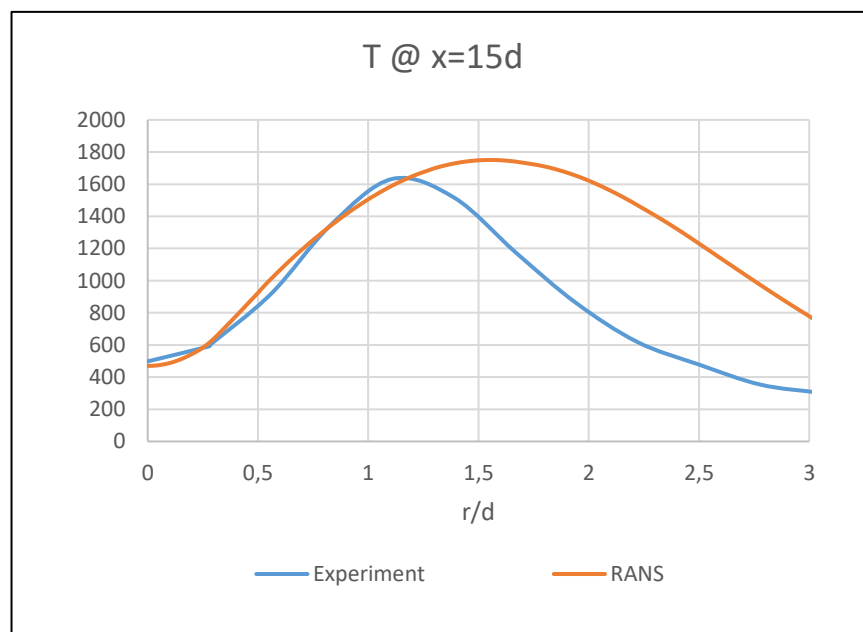


Figure 4. 4. Radial temperature profiles of the Sandia D flame at $x= 15d$.

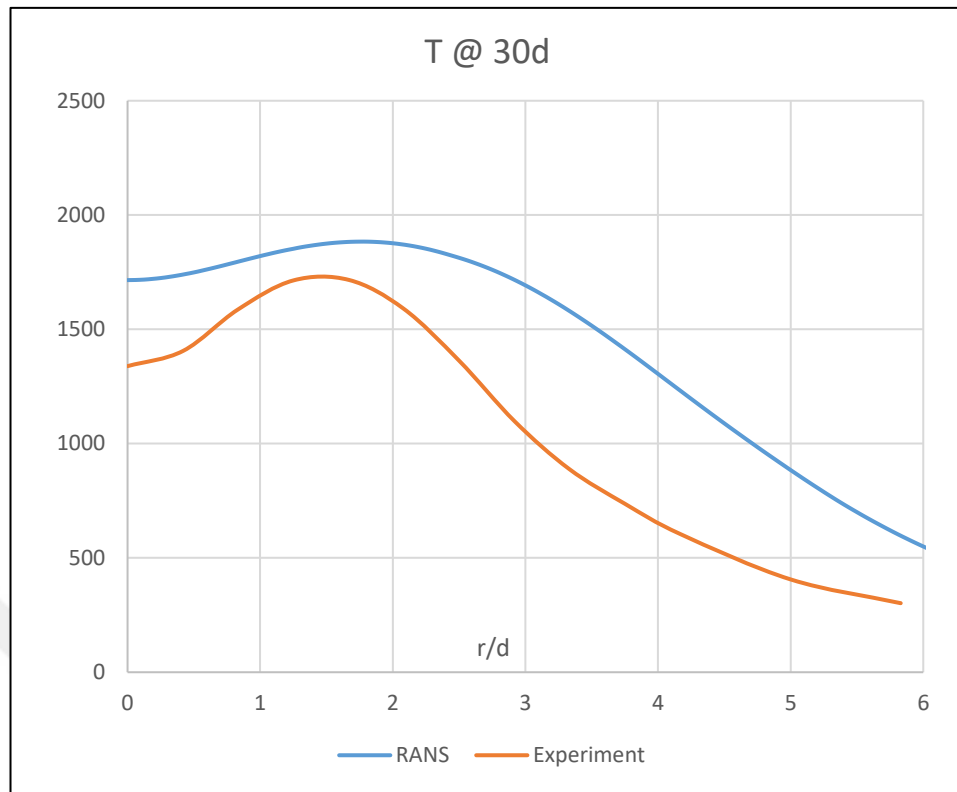


Figure 4. 5. Radial temperature profiles of the Sandia D flame at $x=30d$.

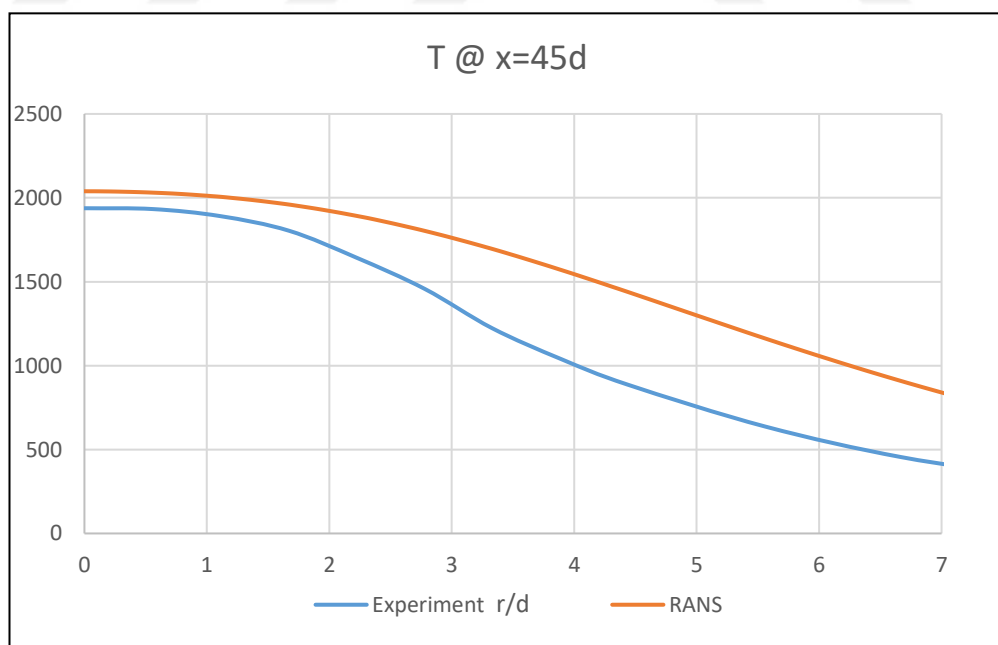


Figure 4. 6. Radial temperature profiles of the Sandia D flame at $x=45d$.

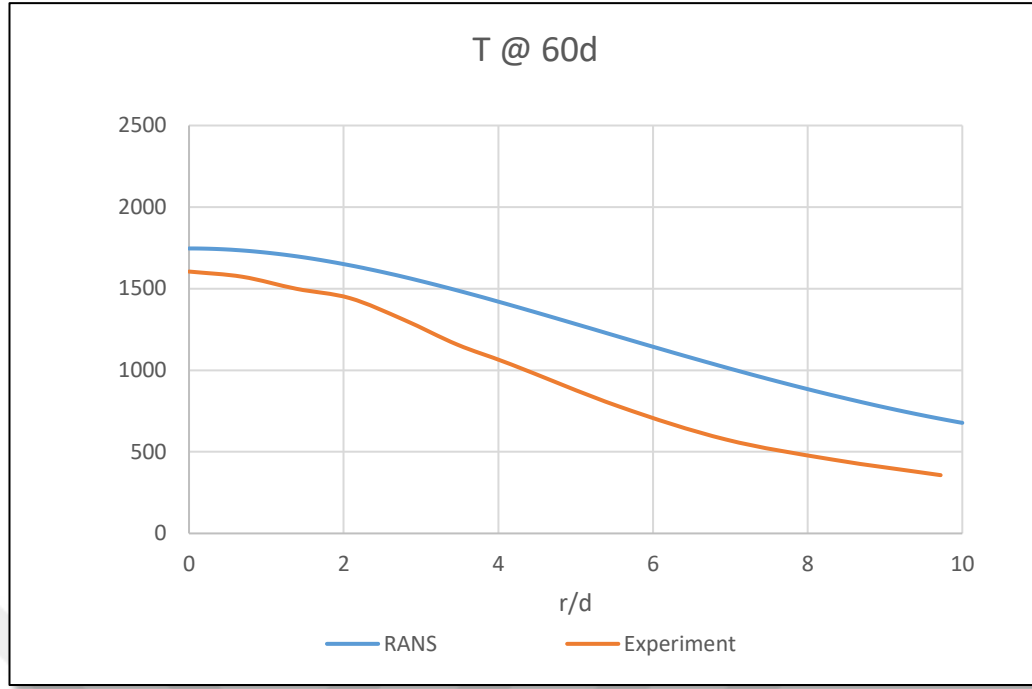


Figure 4. 7. Radial temperature profiles of the Sandia D flame at $x=60d$.

4.2. Oxy Fuel Flame Simulation Details

Geometric dimensions of the computational domain of the Oxy-fuel flames are taken as the same as those of the Sandia D flame. Fuel stream which is composed of 25% CH_4 and 75% oxidizer by volume is fed into the combustion chamber with 49.6 m/s velocity through the central nozzle of the coaxial injector. Pilot stream which surrounds the central nozzle is fed into the combustion chamber with 11.4 m/s velocity. These streams are surrounded by the coflow which has a velocity of 0.9 m/s.

Length of the solution domain in axial direction is taken as 450 mm. A structured mesh with 35000 cells is constructed in the axisymmetric solution domain. Number of cells in the axial and radial directions are taken as 350 and 100, respectively. Mesh is equally spaced in the axial direction, while mesh spacing is increased in the radial direction. A representative structured mesh in the axisymmetric solution domain is plotted below.

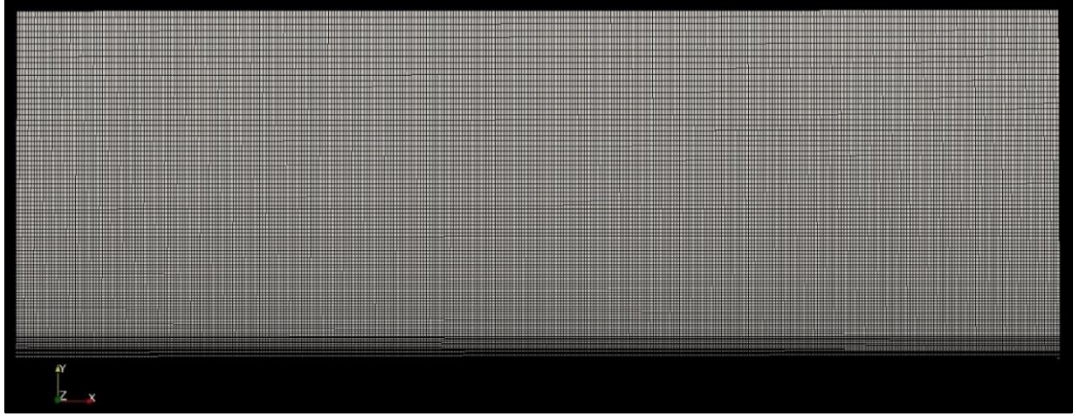


Figure 4. 8: Structured mesh with 35000 cells in the axisymmetric solution domain.

OpenFOAM version 2.1.x is used to simulate Oxy-fuel flame with $k-\epsilon$ turbulence model coupled to SLFM model. Details of the solver can be found in (Müller et al., 2013). Flamelet library is constructed by means of GRI 3.0 chemical mechanism.

4.2.1. Oxy-Fuel Flame Boundary Conditions

Mixture compositions and temperature of the reactants fed into the combustion chamber are listed in the following table. While oxidizer of the Sandia D flame is air, a mixture of O_2+CO_2 with various compositions is the oxidizer of the oxy-fuel flames studied in this thesis. Equivalence ratio of the pilot stream is assumed to be $\Phi=0.77$. Moreover, to study the effects of the temperature of the reactants on flame characteristics, three CFD simulations with the temperature of the reactant streams being 300 K, 500 K, and 700 K are performed.

Table 4. 1: Representative names and compositions of the fuel, pilot and oxidizer streams and the temperature of the reactants.

Representative name of the mixture	Fuel stream	Pilot stream	Coflow/Oxidizer stream	Temperature of the reactants	Mixture fraction of the pilot stream (Z-pilot)
SANDIA D	25% CH ₄ + 75% Air	PHI= 0.77	79% N ₂ + 21% O ₂	300K	0.271
25%	25% CH ₄ + 75% Oxidizer	PHI= 0.77	25% O ₂ + 75% CO ₂	300K	0.314
30% 300K	25% CH ₄ + 75% Oxidizer	PHI= 0.77	30% O ₂ + 70% CO ₂	300K	0.375
30% 500K	25% CH ₄ + 75% Oxidizer	PHI= 0.77	30% O ₂ + 70% CO ₂	500K	0.375
30% 700K	25% CH ₄ + 75% Oxidizer	PHI= 0.77	30% O ₂ + 70% CO ₂	700K	0.375
35%	25% CH ₄ + 75% Oxidizer	PHI= 0.77	35% O ₂ + 65% CO ₂	300K	0.435

At the outer edge of the solution domain, which is parallel to the symmetry axis, inlet velocity of the oxidizer stream (co-flow), 0.9 m/s, is imposed. Therefore, wall turbulence effects are not considered in this thesis. Mixture fraction is set as 1 at fuel inlet and as 0 at oxidizer (co-flow) inlet. Mixture fraction of the pilot stream changes according to its composition as shown in the table given above. At the downstream outlet of the computational domain pressure wave transmissive condition at 1 atm is applied.

5. RESULTS

In this thesis, reactant temperature and different O_2 fraction effects on flame characteristics are studied. Results of three simulations with 30%, 25% and 35% volume fraction of O_2 in the oxidizer stream are presented to investigate the effects of CO_2 dilution on combustion. Furthermore, for 30% O_2 volume fraction case, results of three simulations with the inlet temperature of the reactant streams being 300 K, 500 K and 700 K are presented to understand the influence of the reactants' temperature on combustion.

5.1. 2-D Counterflow Diffusion Flame Results

2-D counterflow diffusion flame is calculated in the mixture fraction space. By increasing mass flow rate at constant domain length, strain rate effects on the flame chemistry and temperature can be investigated. GRI 3.0 chemical kinetics mechanism is used to calculate flamelets. As shown in the table below, oxidizer streams with various O_2 volume fractions are considered. Fuel mixture consists of 25% CH_4 and 75% oxidizer by volume. Fuel mixture is represented by $Z=1$. This mixture is burned with pure oxidizer. Oxidizer is represented by $Z=0$. Volume fraction of O_2 in the oxidizer may vary. In the table given below, for each case of O_2 fraction in the oxidizer stream, stoichiometric mixture fraction is listed.

Table 5. 1: Mixture fractions at stoichiometric conditions.

Case Name	Z stoichiometric
25%	0.404
30%	0.480
35%	0.556

5.1.1. O₂ Fraction Effects on the Flame

Temperature distributions according to mixture fraction for various strain rates are plotted below. As seen from the figures, resistance of the reaction to strain rates increases as O₂ volume fraction gets higher. While extinction limit is reached at 33.7 1/s strain rate for 25% O₂ in the oxidizer mixture, extinction limit is reached at 157 1/s strain rate for 30% O₂ in oxidizer mixture. Extinction limit reaches its maximum value at a strain rate of 355 1/s, for 35% O₂ in the oxidizer mixture. Flame temperature increases as O₂ fraction is increased.

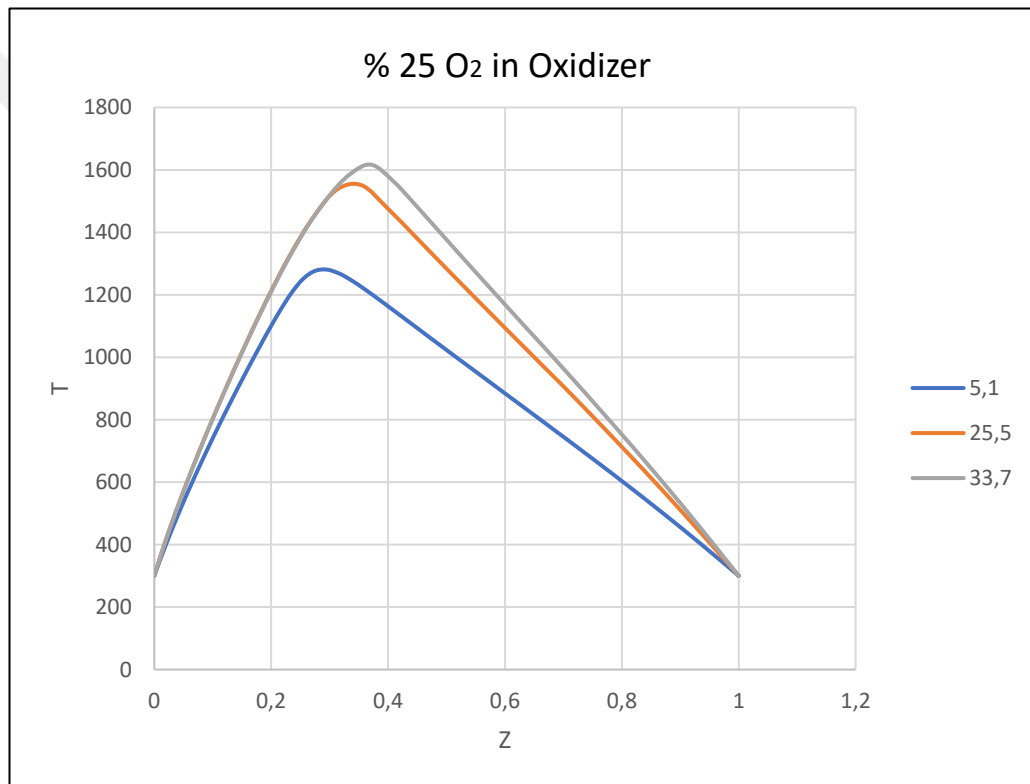


Figure 5. 1: Temperature distribution according to mixture fraction for 25% O₂ volume fraction in the oxidizer.

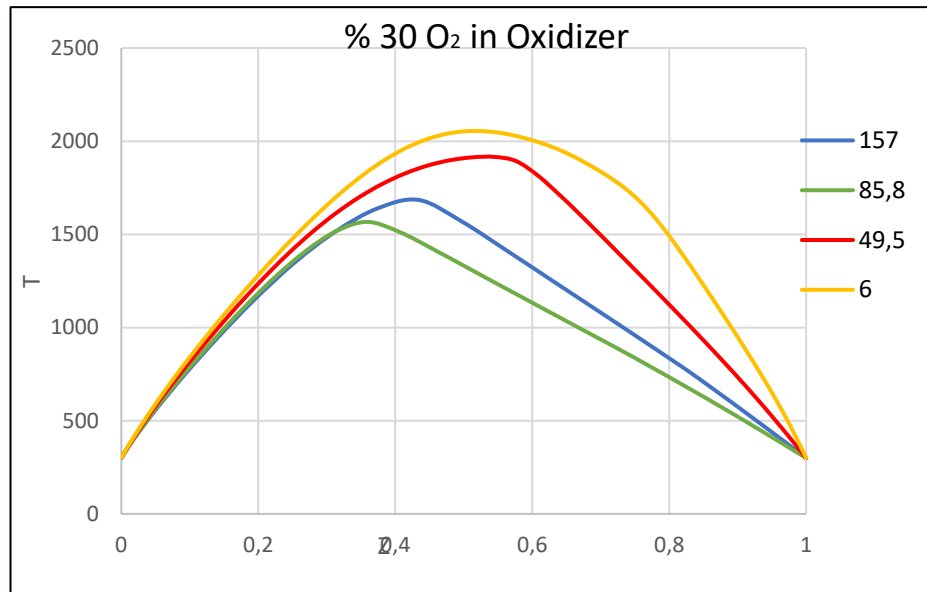


Figure 5. 2. Temperature distribution according to mixture fraction for 30% O_2 volume fraction in the oxidizer.

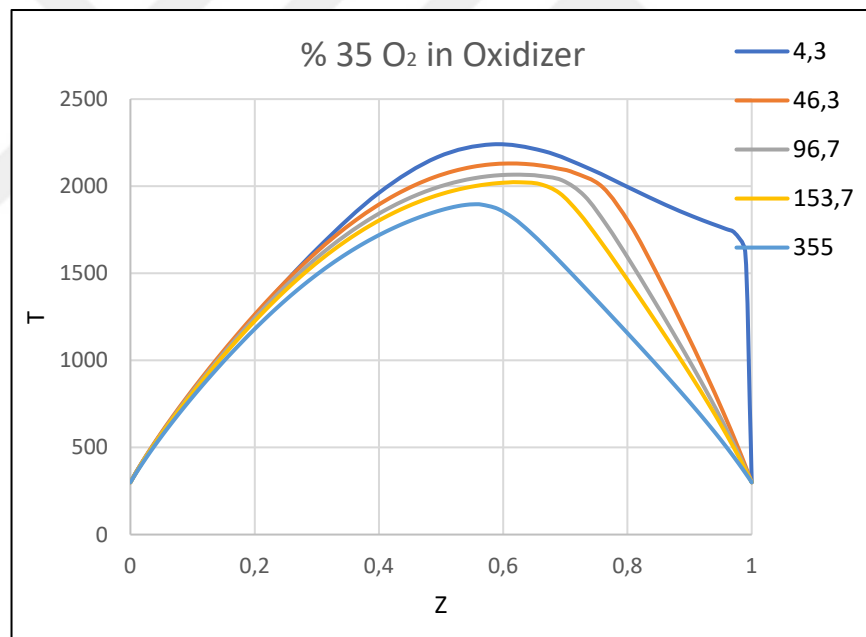


Figure 5. 3: Temperature distribution according to mixture fraction for 35% O_2 volume fraction in the oxidizer.

OH production distributions according to mixture fraction for various strain rates are plotted below. OH production starting and termination points indicate the extent of the reaction sheet. As the volume fraction of O_2 is increased thickness of the reaction sheet, i.e flame is enlarged. Moreover, increased O_2 fraction in the oxidizer mixture

increases OH production level which can be attributed to higher flame temperature caused by increased reaction rate due to elevated O_2 fraction.

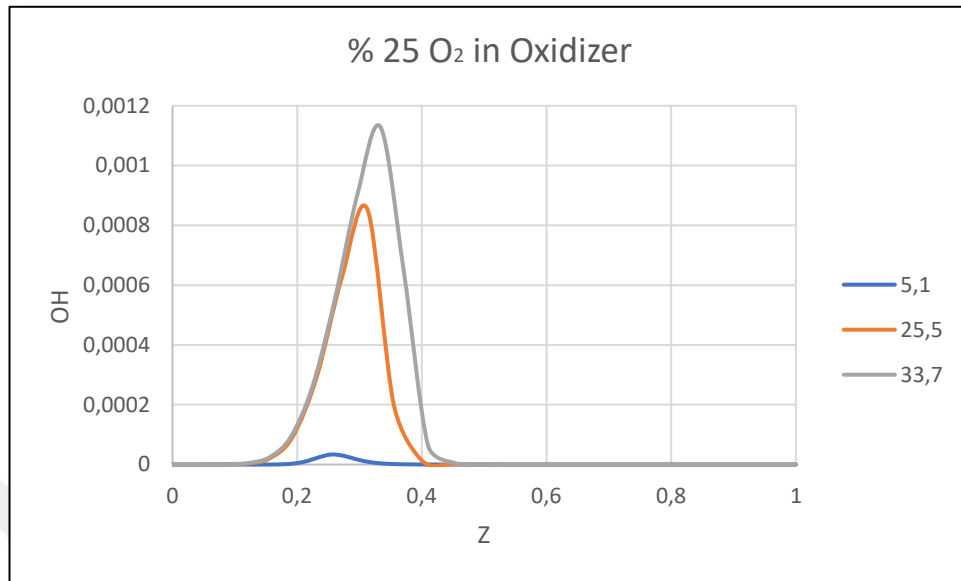


Figure 5. 4: OH production distribution according to mixture fraction for 25% O_2 volume fraction in the oxidizer.

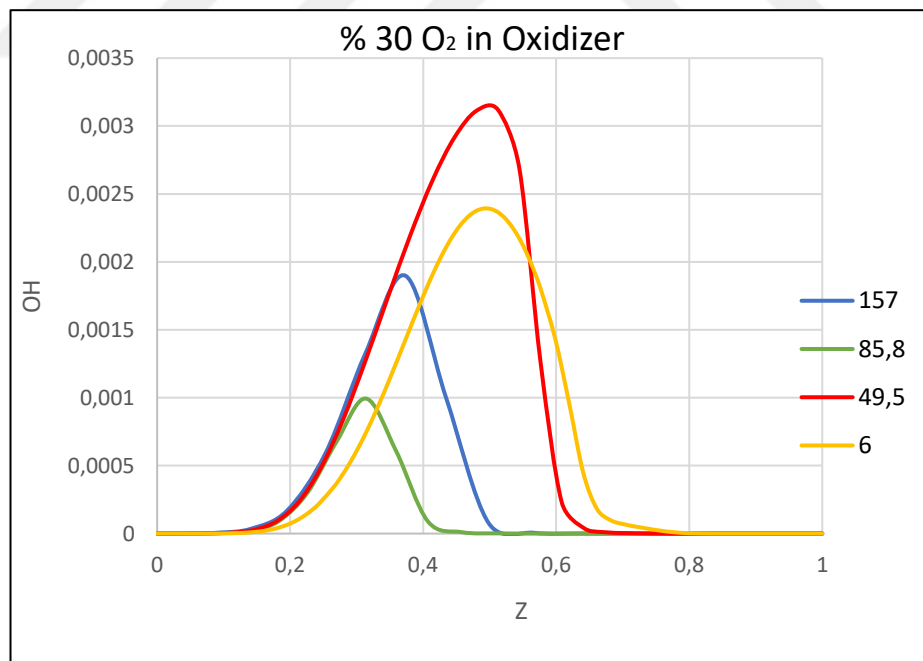


Figure 5. 5: OH production distribution according to mixture fraction for 30% O_2 volume fraction in the oxidizer.

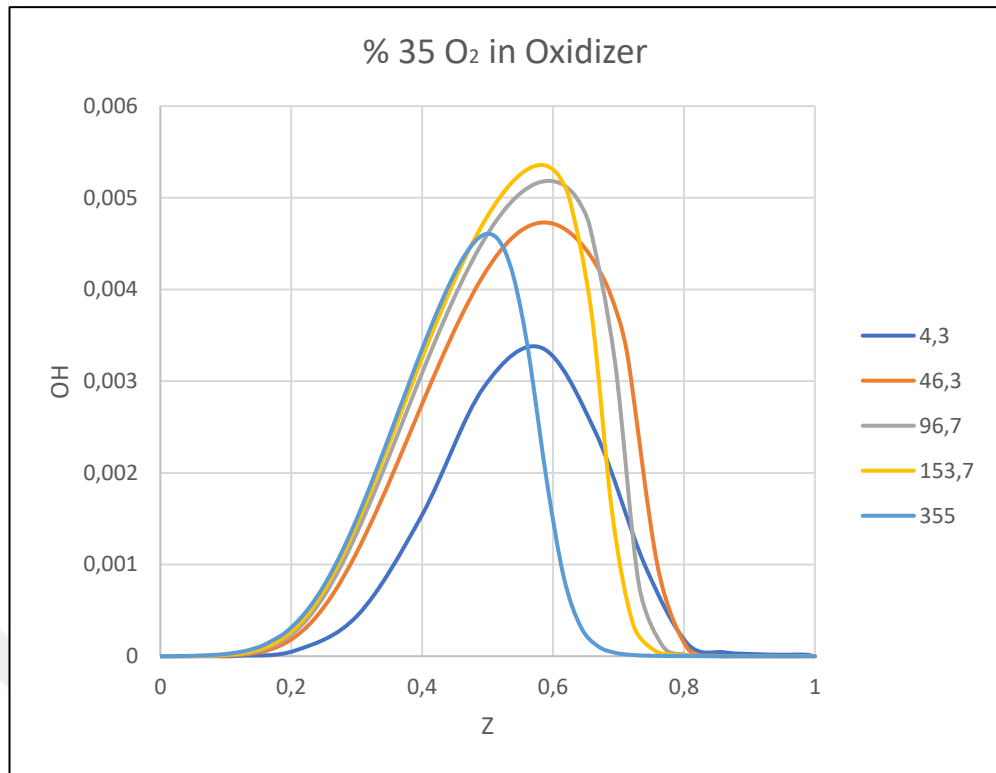


Figure 5. 6: OH production distribution according to mixture fraction for 35% O₂ volume fraction in the oxidizer.

5.1.2. Reactant Inlet Temperature Effects on Flame Characteristics

Temperature distributions according to mixture fraction for various strain rates at several reactant inlet temperatures are shown below. Increasing temperature of the reactants cause enhanced resistance of the reaction against strain rate. While for 300 K reactant temperature extinction limit is reached at 157 1/s strain rate, for 700 K reactant temperature extinction limit is reached at 959 1/s strain rate. Extinction limit reaches its maximum value for a strain rate of 11414.3 1/s for 500 K inlet temperature of the reactants. Flame temperature increases as the temperature of the reactants is increased.

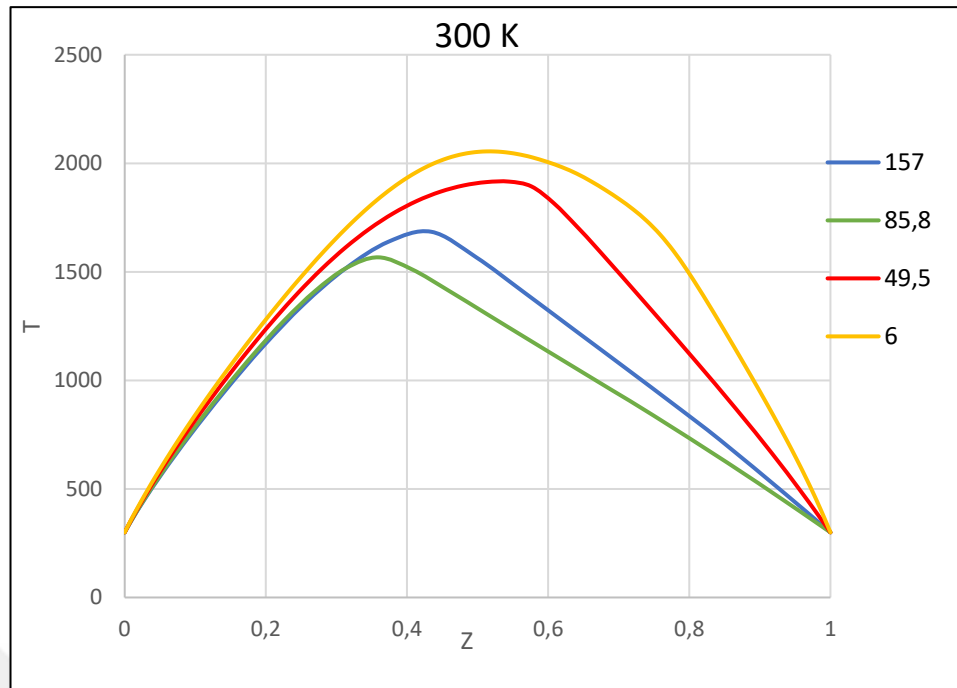


Figure 5. 7: Temperature distribution according to mixture fraction for reactants' inlet temperature of 300K.

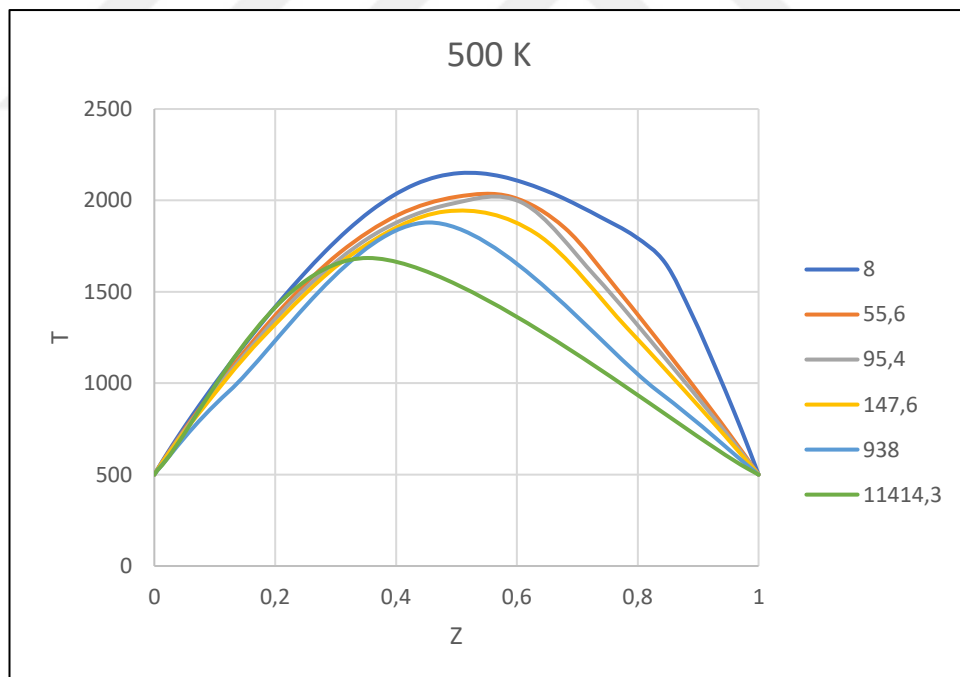


Figure 5. 8: Temperature distribution according to mixture fraction for reactants' inlet temperature of 500K.

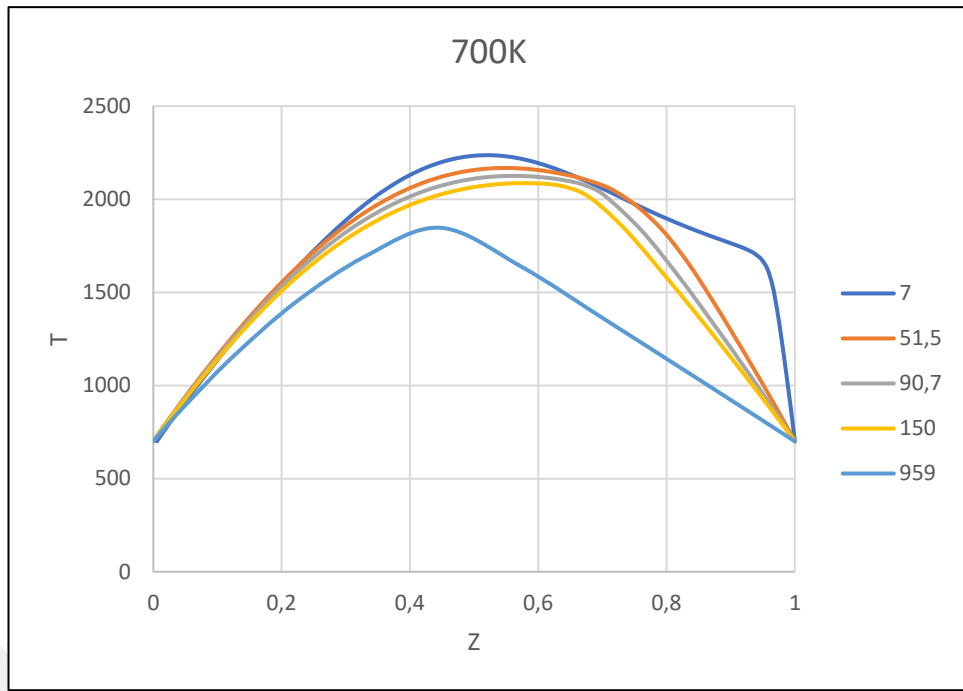


Figure 5. 9: Temperature distribution according to mixture fraction for reactants' inlet temperature of 700K.

OH mass fraction distributions according to mixture fraction for various strain rates at several reactant inlet temperatures are plotted below. OH production starting and terminating points indicate the extent of the reaction sheet. Increased reactant temperature cause enlargement of the reaction sheet thickness, namely the flame thickness. Moreover, OH production increases as the temperature of the reactants is increased which can be attributed to higher flame temperature caused by increased reaction rate.

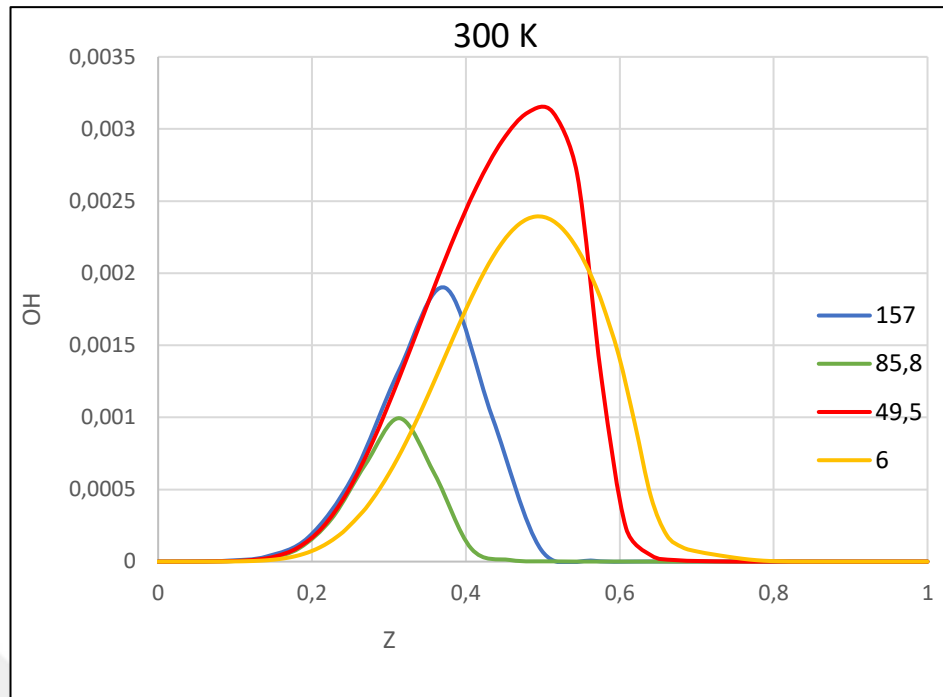


Figure 5. 10: OH mass fraction distribution according to mixture fraction for reactants' inlet temperature of 300K.

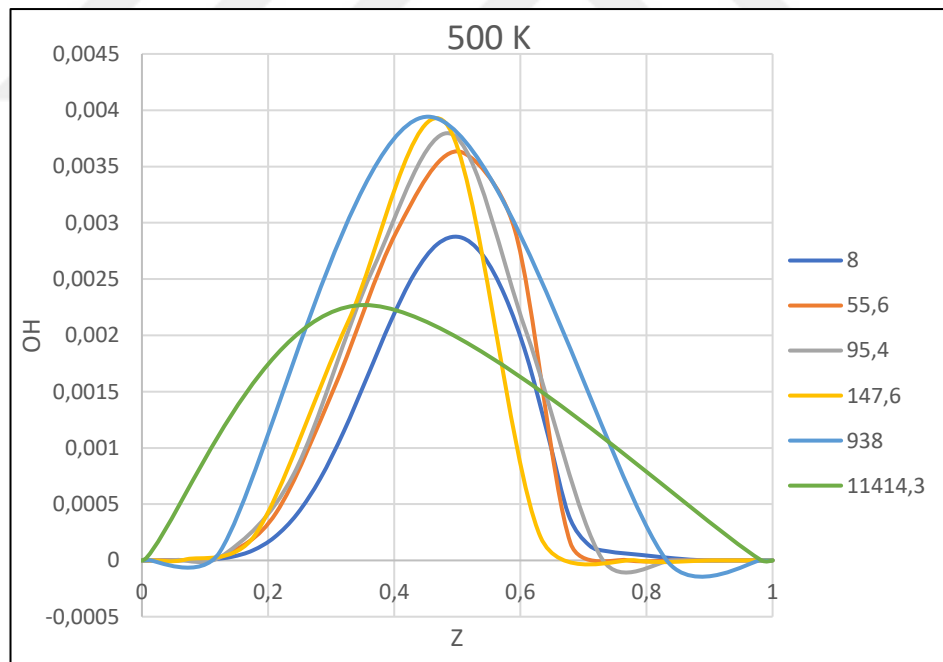


Figure 5. 11: OH mass fraction distribution according to mixture fraction for reactants' inlet temperature of 500K.

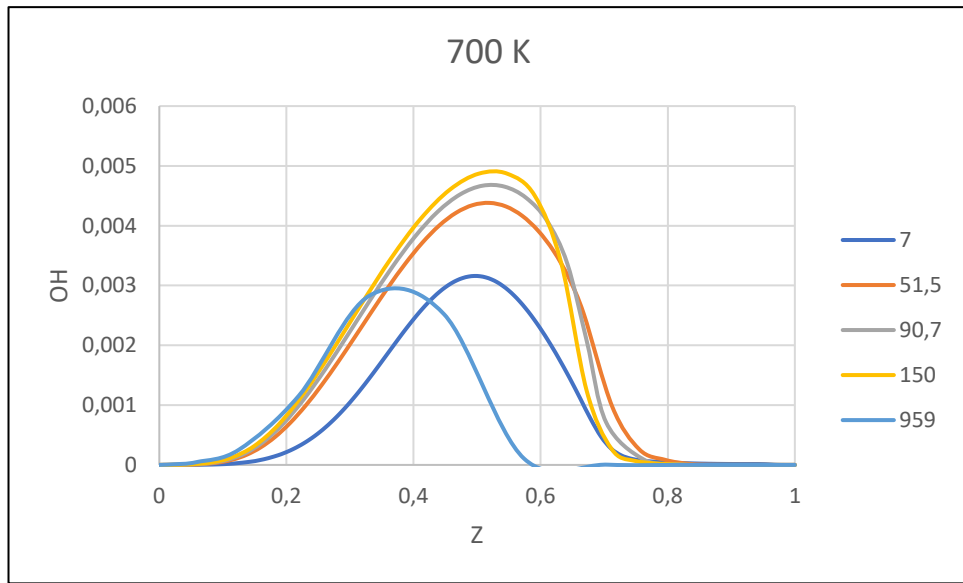


Figure 5. 12: OH mass fraction distribution according to mixture fraction for reactants' inlet temperature of 700K.

5.2. RANS Simulation Results

Changes in O_2 volume fraction of the oxidizer stream and the temperature of the reactants influences mixture thermodynamic (such as density, specific heat and enthalpy) and transport (momentum, thermal and mass diffusivities) properties. Some of these changes are listed in the following table. By increasing the temperature of the reactants, dynamic viscosity of the fuel mixture increases, while fuel mixture density decreases. For a specified fuel stream inlet velocity, these changes lead to an increase in mass and momentum flow rates as well as the Reynolds number of the fuel jet as the temperature of the reactants is decreased, which in turn increase the penetration length of the fuel jet. Furthermore, specific heat of the fuel mixture increases as the temperature of the reactants is decreased so that heat capacity rate of the fuel stream increases.

Table 5. 2: Fuel mixture thermal and transport properties.

O ₂ volume fraction in oxidizer mixture (O ₂ +CO ₂)	Reactant temperature	Fuel viscosity (μPa-s)	Density (kg/m ³)	Reynolds number	Momentum	Fuel mass flow rate (kg/s)	Specific heat Cp (kJ/m ³ -K)
30%	300K	15.777	1.3976	31635	0.1399	0.0028	1.435
30%	500K	24.697	0.8366	12097	0.0838	0.0017	1.026
30%	700K	32.242	0.5973	6616	0.0598	0.0012	0.835
25%	300K	15.557	1.4162	32509	0.1418	0.0029	1.447
35%	300K	16.000	1.3790	30779	0.1381	0.0028	1.422

Therefore, as seen in the temperature contour plots below, flame length increases with decreasing temperature of the reactants due to increased momentum flow rate of the fuel stream for decreased temperature of the reactants. Furthermore, location of the peak flame temperature curve gets closer to the symmetry axis, and it is extended further downstream as the temperature of the reactants is decreased.

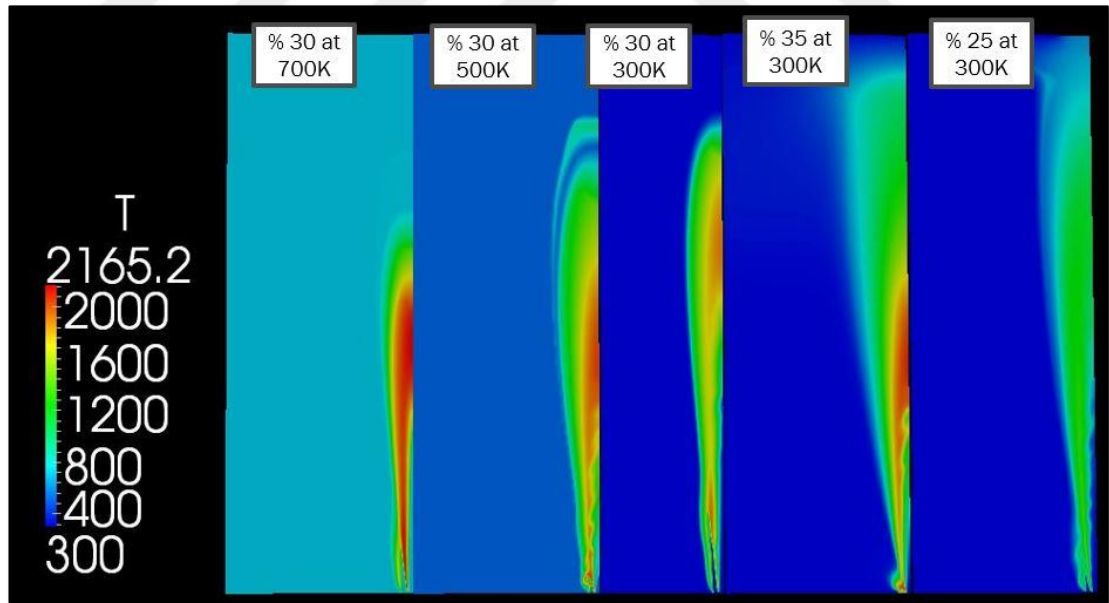


Figure 5. 13: Temperature contours of the flames.

On the other hand, if cases with the same inlet temperature of the reactants, 300 K, but with different O₂ volume fractions in the oxidizer stream are compared, near field peak flame temperatures are significantly higher at any axial position and the

peak temperature zone is located closer to the injector and symmetry axis as well for O_2 volume fraction of 35% case as compared to the one with 25%. However, comparison of cases with different O_2 fractions shows that the difference in flame lengths is not significant due to small difference in their momentum flow rates. Furthermore, for O_2 volume fraction of 35% case flame penetrates further in the radial direction as compared to the 25% case due to its smaller momentum flow rate. However, reaction temperature decreases significantly by increasing CO_2 dilution (decreasing the O_2 volume fraction from 35% to 25%) of the oxidizer stream. CO mass fraction contour plots obtained by CFD simulations of various cases are presented below. For the case of reactants' inlet temperature of 300 K and O_2 volume fraction of 25% in the oxidizer stream, flame temperature is rather low and CO contour plot points out that that flame blows off due to insufficient oxygen content of the oxidizer stream. In this case significant amount of CO formed by incomplete combustion diffuses outward in the radial direction. Among the cases considered in this thesis, least CO production occurs in the case of reactants' inlet temperature of 300 K and O_2 volume fraction of 35% in the oxidizer stream. Furthermore, as seen from the contour plots below, re-production of CO does not occur in this case. Therefore, the piloted oxy-fuel diffusion flame formed by reactants with inlet temperature of 300 K and a CO_2 diluted oxidizer stream with O_2 volume fraction of 35% results in satisfactory reduction in CO emissions.

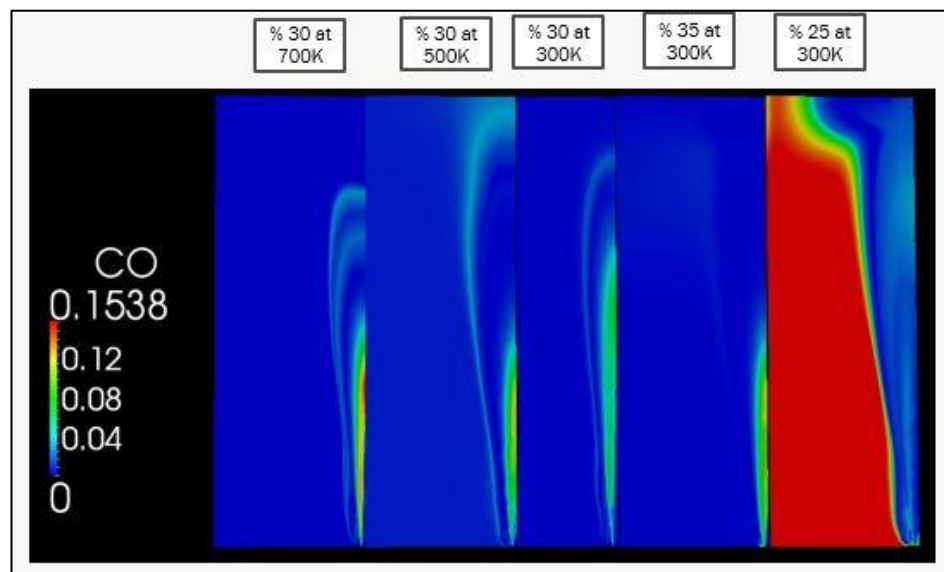


Figure 5. 14: CO mass fraction contours of the flames.

For cases considered in this thesis, peak flame temperature data are listed in the following table. By increasing the temperature of the reactants and O₂ volume fraction, peak flame temperature increases. Comparison of 35% O₂ case with 30% O₂ and 700 K reactants' temperature case, 35% O₂ in the oxidizer mixture is better in controlling the flame temperature. Although, flame length increases as the O₂ volume fraction is increased, CO production ceases before the flame reaches the exhaust of the combustion chamber. On the other hand, elevating the inlet temperature of the reactants to 700 K causes re-production of CO in the far field at the downstream of the main diffusion flame.

Table 5. 3: Peak flame temperatures.

O2 volume fraction in the oxidizer stream	30%			35%	25%
Temperature of the reactants	700 K	500 K	300 K	300 K	300 K
Peak flame temperature	2165 K	2038 K	1931 K	2082 K	1424 K

Temperature of the reactants which influences thermodynamic and transport properties of the reacting mixture is an important parameter in analyzing flame stability. Density and viscosity changes influence momentum and mixing characteristics of fuel jets, while changes in the specific heat of the mixture causes variations in flame temperature. Flame resistance against aerodynamic strain can be determined by analyzing the coupled effects of these changes on flame characteristics.

Axial temperature distributions for cases with various O₂ volume fractions of the oxidizer stream and inlet temperature of the reactants are presented in the following figure. In case with 30% O₂ volume fraction in the oxidizer and reactants' inlet temperature of 300 K, peak temperature of 1900 K occurs at $x/d=43$ in the far field significantly away from the injector due to delayed mixing of the fuel with enough oxidizer for high momentum flow rate of the fuel stream. Similarly, in 25% O₂ fraction with the same inlet temperature of the reactants case, a significantly lower peak temperature of 1130 K occurs at $x/d=41$ in the far field significantly away from the injector, approximately at the same location as before. In these two cases, sufficient mixing of the fuel and oxidizer streams because of shear layer instability is realized quite away from the injector due to the same momentum flow rates of the fuel streams

in both cases. However, in 25% O₂ volume fraction case, excessive dilution of the oxidizer stream with CO₂ causes significantly increased CO production because of incomplete combustion and eventual flame blow off.

In the case of 30% O₂ volume fraction in the oxidizer stream and reactants' inlet temperature of 700 K, mixing of the fuel and oxidizer streams progresses more rapidly and therefore sufficient mixing is completed much closer to the injector due to significantly lower momentum flow rate of the fuel jet as compared to the previous two cases which is caused by considerably higher inlet temperature of the reactants in the final case, resulting in peak flame temperature of 2165 K at $x/d=29$. In this case reaction occurs earlier as compared to the previous two cases because of considerably higher inlet temperature of the reactants. However, the mixing is insufficient to anchor the flame to the injector.

In cases with 35% O₂ volume fraction in the oxidizer stream and reactants' inlet temperature of 300 K and 30% O₂ volume fraction in the oxidizer stream and reactants' inlet temperature of 500 K, flame can be anchored to the injector. In both cases stratification is not observed in the fuel jet. Oxidizer entrainment to the fuel stream next to the injector enhances mixing. This well-mixing behavior is desired for stable operation. In both cases locations, $x/d=25.6$ and $x/d=25.6$, respectively, and values of the peak temperatures, 2081 K and 2032 K, respectively, which are both slightly smaller than that of the 700 K reactant temperature and 30% O₂ volume fraction case, are close to each other.

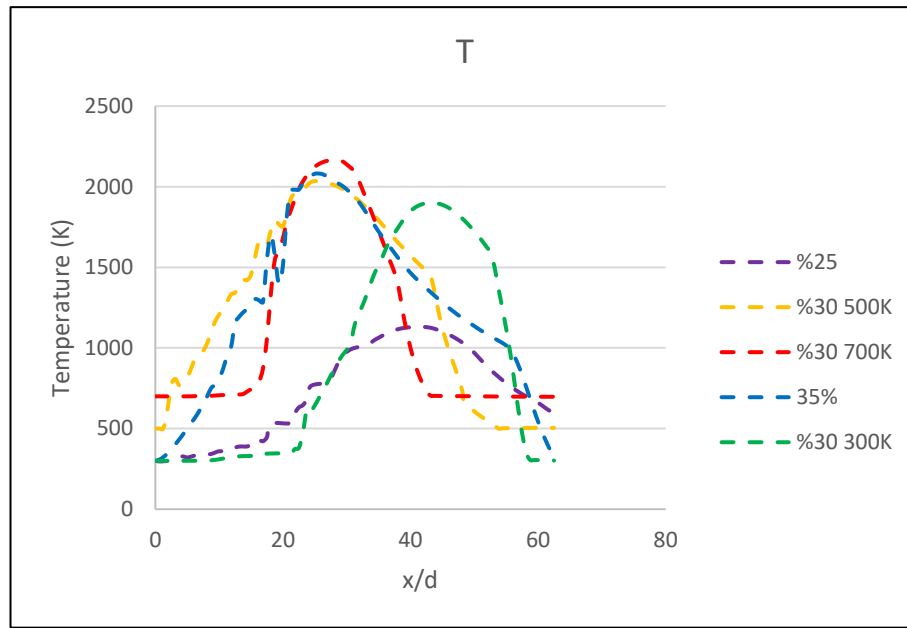


Figure 5. 15: Axial temperature distributions for various O₂ volume fractions of the oxidizer and reactants' inlet temperatures.

CO distributions along the symmetry axis x for the cases considered in this thesis are presented in the following figure. As seen from the Figures 5.16 and 5.15, CO and temperature distributions along the symmetry axis can be approximately correlated. In all 30% O₂ volume fraction cases considered CO recombination reactions occur in a single region or in multiple regions surrounding the main flame as seen in Figures 5.14 and 5.16 which cause incompletely burned combustion products leave the combustion chamber. However, no incomplete combustion products exist at the outlet of the combustion chamber for a flame generated by the reaction of the fuel and oxidizer with 35% O₂ volume fraction which is satisfactory for emissions reduction.

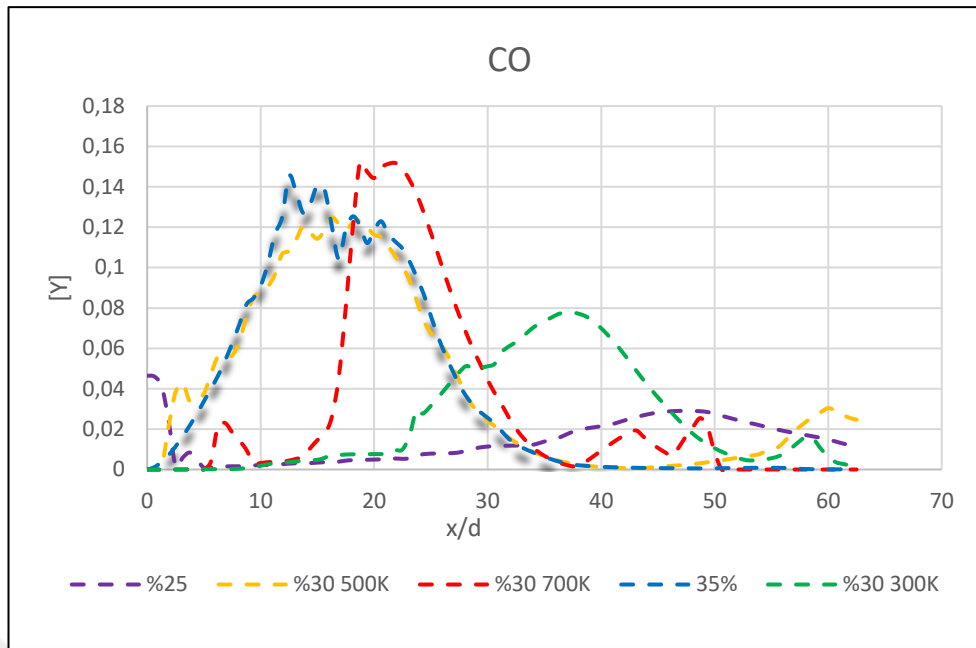


Figure 5. 16: Axial CO mass fraction distributions for various O₂ volume fractions of the oxidizer and reactants' inlet temperatures.

For the case of reactants' inlet temperature of 300K, temperature and species mass fraction distributions in radial direction at $x= 15d$, $x= 30d$ and $x= 45d$ locations are given in Figures 5.17, 5.18 and 5.19, respectively, where $d= 7.2$ mm is the diameter of the fuel nozzle.

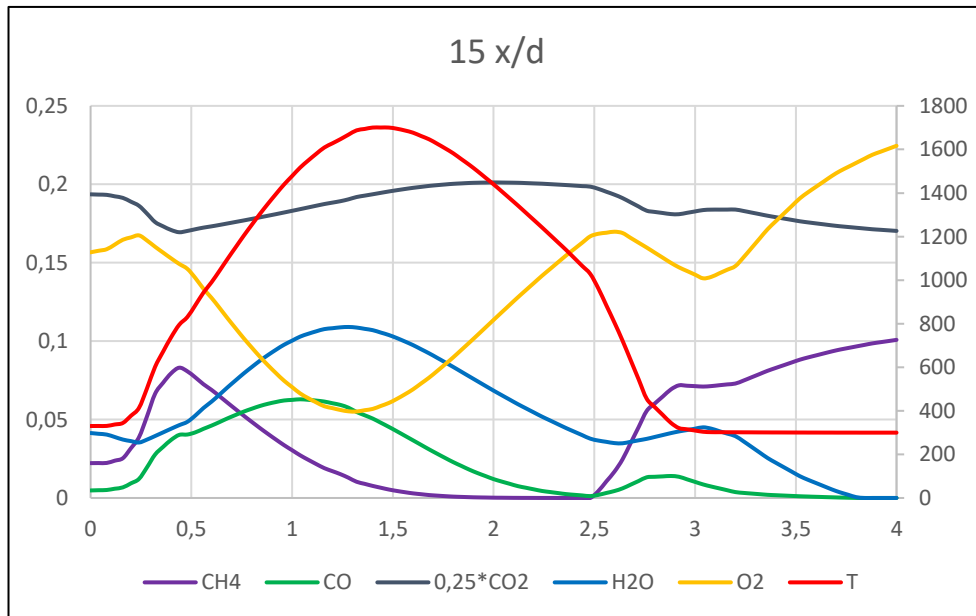


Figure 5. 17: Radial distributions of species mass fractions and flame temperature at $x=15d$ for reactants' inlet temperature of 300K.

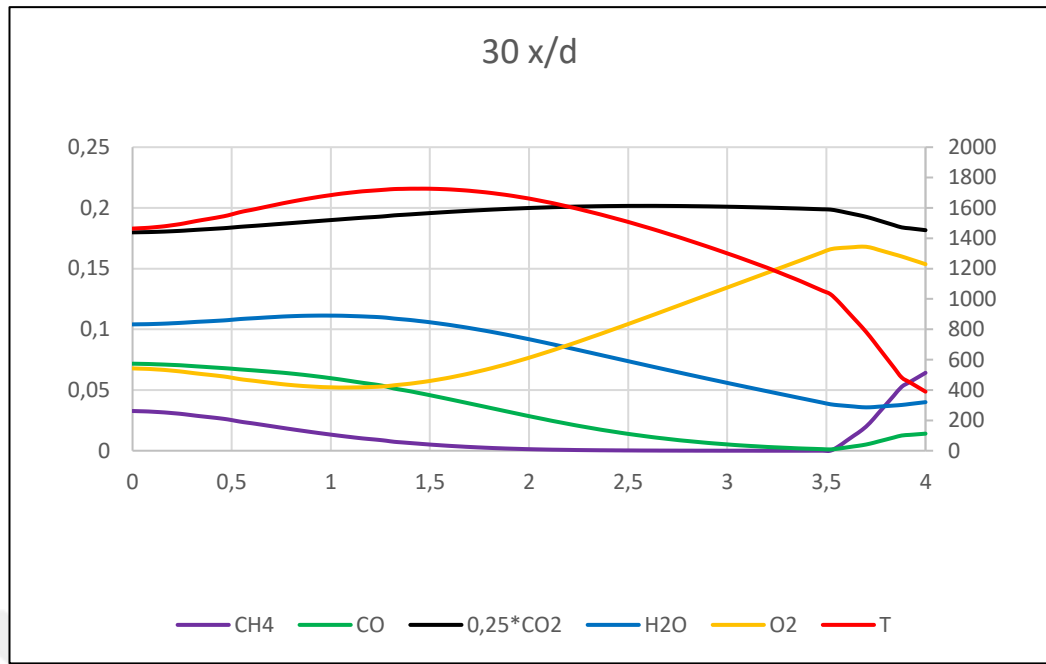


Figure 5. 18: Radial distributions of species mass fractions and flame temperature at $x=30d$ for reactants' inlet temperature of 300K.

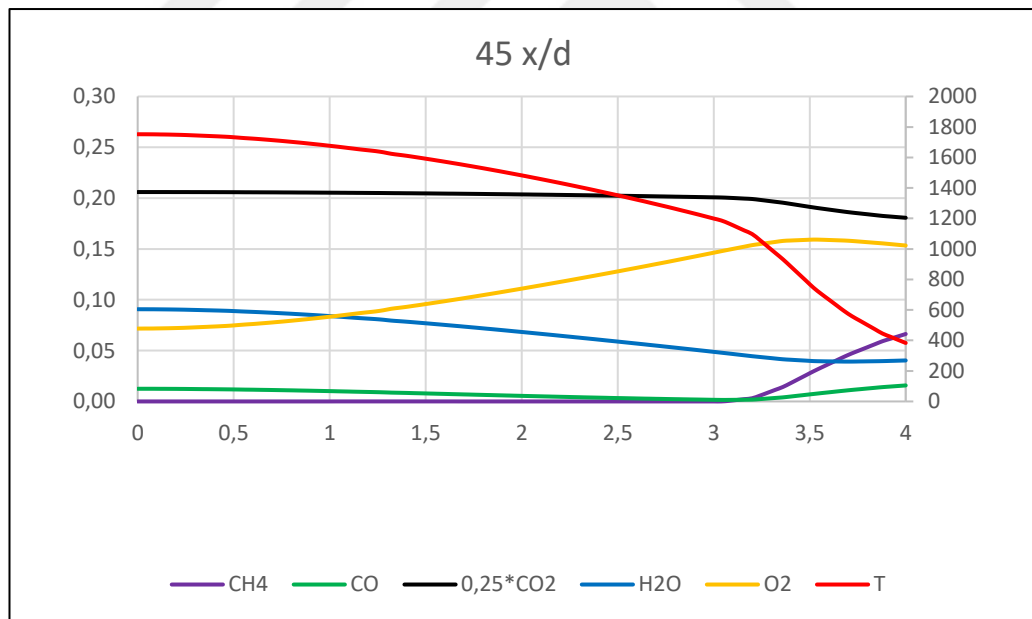


Figure 5. 19: Radial distributions of species mass fractions and flame temperature at $x=45d$ for reactants' inlet temperature of 300K.

For the case of reactants' inlet temperature of 500K, temperature and species mass fraction distributions in radial direction at $x= 15d$, $x= 30d$ and $x= 45d$ locations are given in Figures 5.20, 5.21 and 5.22, respectively. For this case flame spreads further in the radial direction due to its smaller momentum flow rate as compared to the

previous case of 300 K inlet temperature, which results in more gradual decrease of the flame temperature in the radial direction as compared to that for the corresponding axial station of the previous case, which can also be seen in Figure 5.13. Therefore, flammable area is broader in this case.

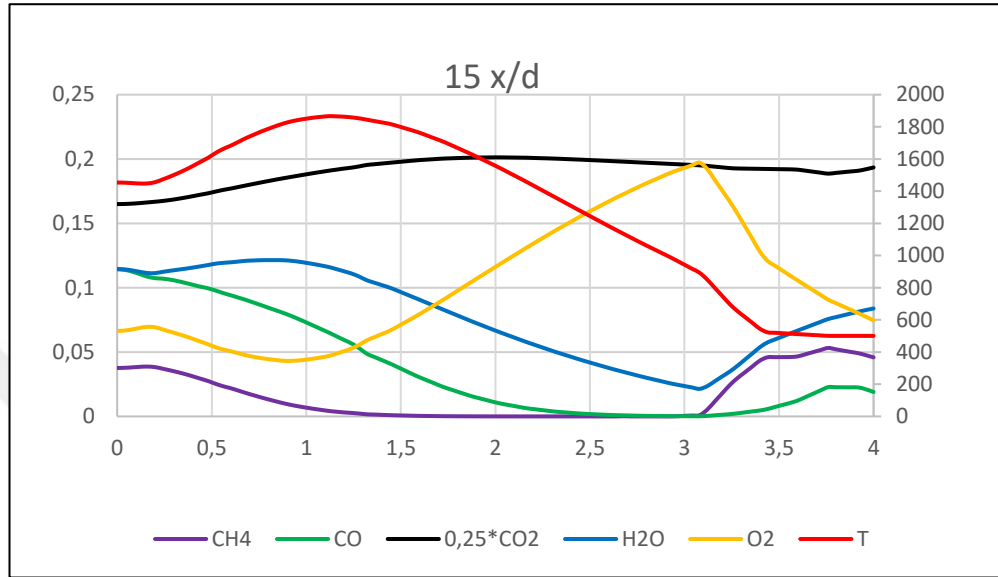


Figure 5. 20: Radial distributions of species mass fractions and flame temperature at $x=15d$ for reactants' inlet temperature of 500K.

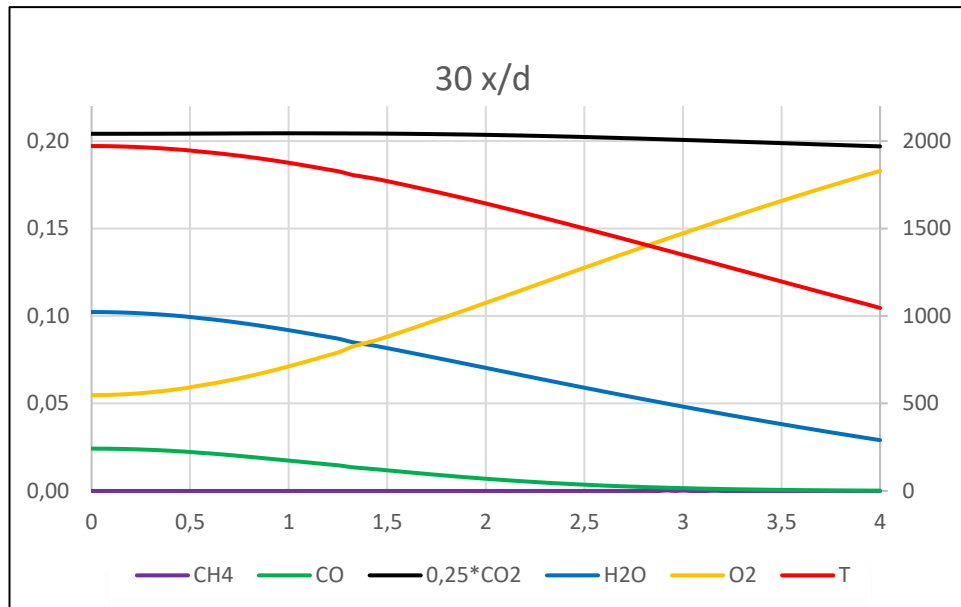


Figure 5. 21: Radial distributions of species mass fractions and flame temperature at $x=30d$ for reactants' inlet temperature of 500K.

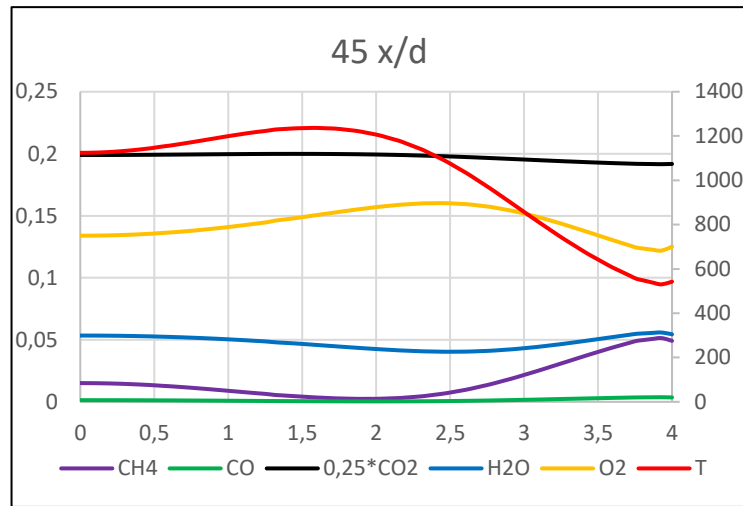


Figure 5.22: Radial distributions of species mass fractions and flame temperature at $x=45d$ for reactants' inlet temperature of 500K.

For the case of reactants' inlet temperature of 700K, temperature and species mass fraction distributions in radial direction at $x= 15d$, $x= 30d$ locations are given in Figures 5.23 and 5.24, respectively. While increasing the temperature of the reactants enlarges the flammability limits, i.e shifting lower and upper flammability limits to a leaner and richer mixture, respectively, besides decreased flame length, in a plane normal to the symmetry axis flame area becomes smaller for reactants' inlet temperature of 700 K than that for the 500 K case.

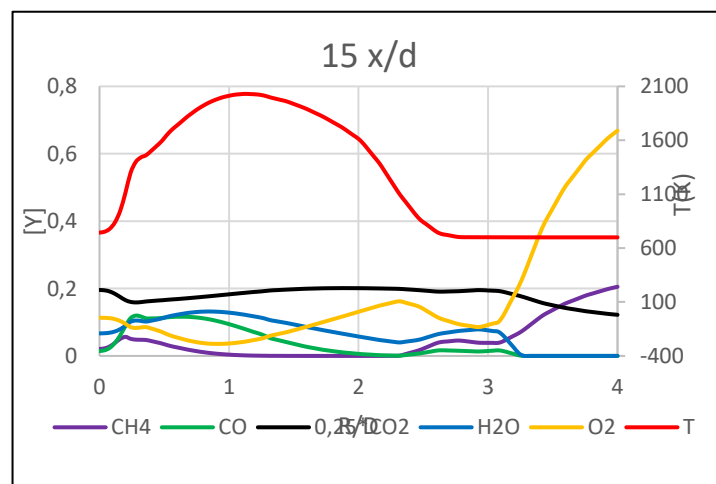


Figure 5.23: Radial distributions of species mass fractions and flame temperature at $x=15d$ for reactants' inlet temperature of 700K.

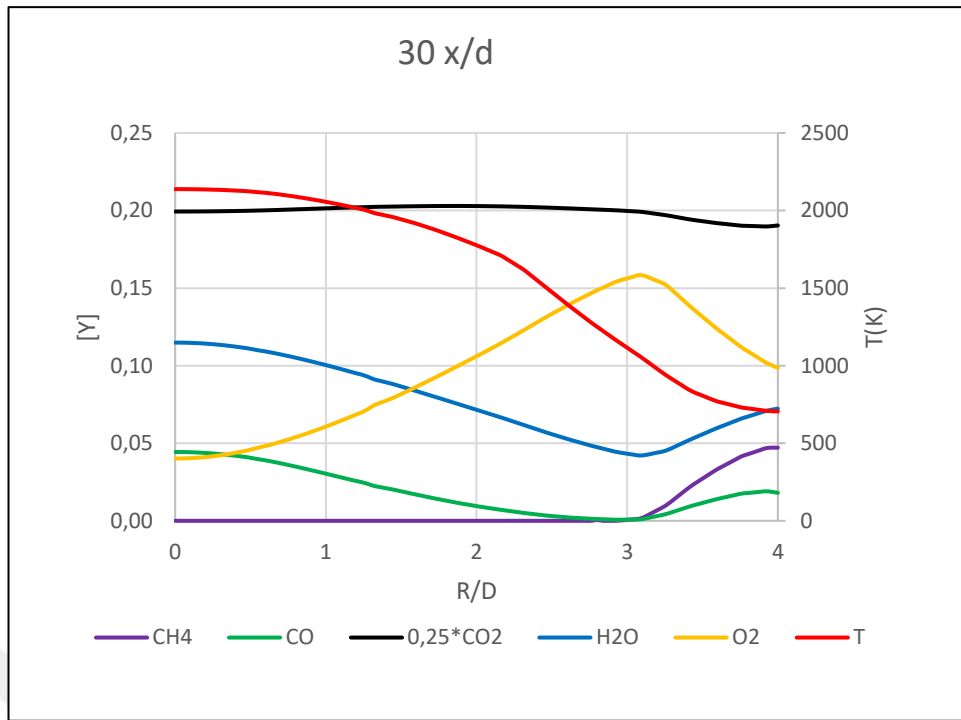


Figure 5. 24: Radial distributions of species mass fractions and flame temperature at $x=30d$ for reactants' inlet temperature of 700K.

Radial distributions of the flame temperature at various axial locations for reactants' inlet temperatures of 300K, 500 K and 700 K are given in Figures 5.25, 5.26 and 5.27, respectively. These distributions show that increased temperature of the reactants causes decay of the flame temperature in a shorter distance in axial direction. Near the injector temperature gradient is sharp for the reactants' temperature of 300 K case which causes stratification and slow mixing of the fuel and pilot streams. Therefore, flame length increases if the temperature of the reactants is decreased. Increased temperature of the reactants leads to better mixing of the fuel and oxidizer streams, resulting in shorter flame length for the 500 K reactants' inlet temperature case as compared to that for the 300 K case.

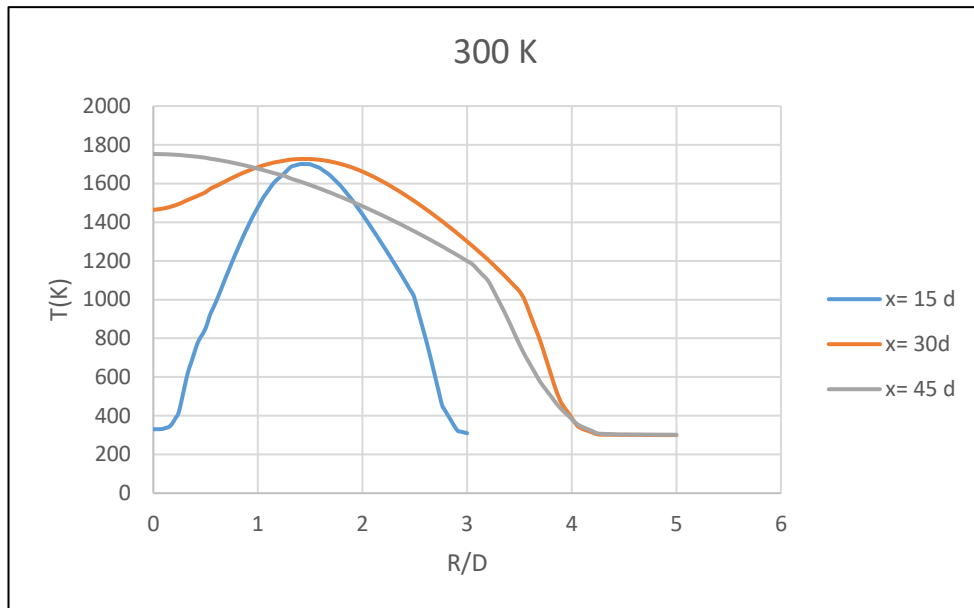


Figure 5. 25: Radial distributions of the flame temperature at various axial locations for reactants' inlet temperature of 300K.

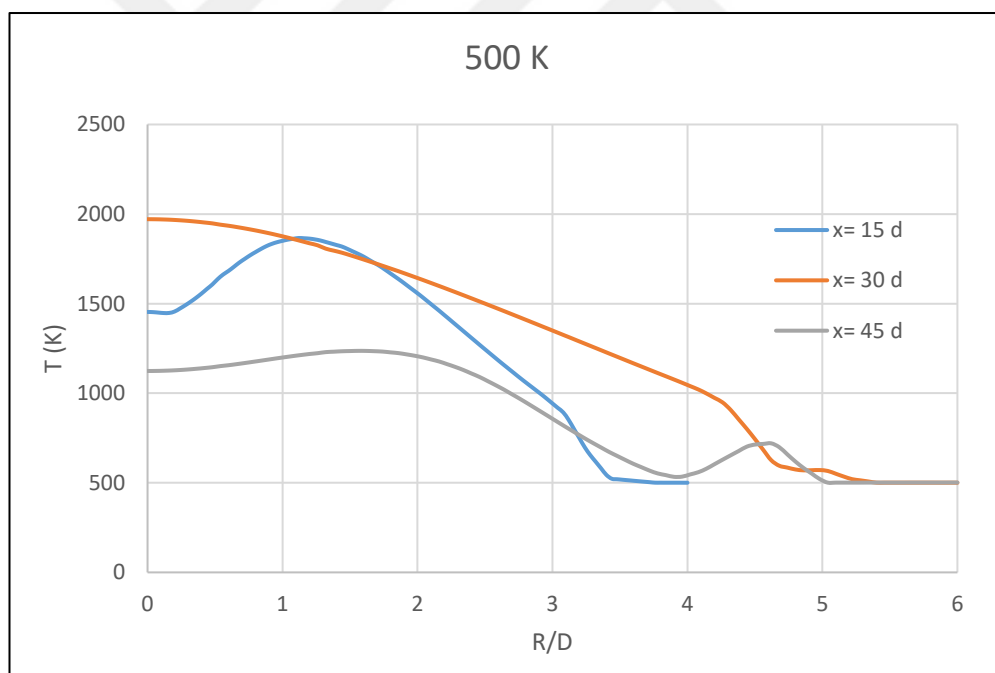


Figure 5. 26: Radial distributions of the flame temperature at various axial locations for reactants' inlet temperature of 500K.

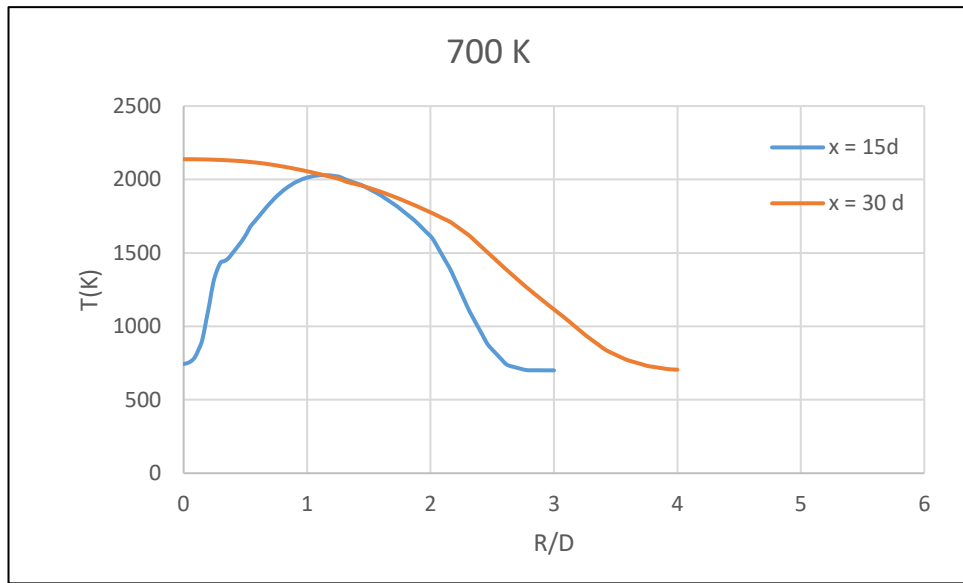


Figure 5. 27: Radial distributions of the flame temperature at various axial locations for reactants' inlet temperature of 700K.

Furthermore, both flame width and length are smaller than those of the previous two cases considered as the temperature of the reactants is increased further to 700 K, which can be attributed to increased reactivity and flame temperature.

Dilution of O_2 with CO_2 influences thermodynamic and transport properties of the combustible mixture. By decreasing CO_2 dilution, namely increasing O_2 fraction in the oxidizer stream, density, and momentum of the fuel jet decreases. Flame temperature profiles in radial direction at various axial locations are presented for O_2 volume fractions of 25% and 30%, in Figures 5.28 and 5.29, respectively. Comparison of the figures reveals that at the edge of the flame temperature gradients in radial direction are sharper if O_2 volume fraction of the oxidizer stream is increased which can be attributed to increased reaction rate and decreased turbulent thermal diffusivity of the shear layer between the fuel and oxidizer streams. Furthermore, flame temperature is higher if CO_2 dilution is decreased.

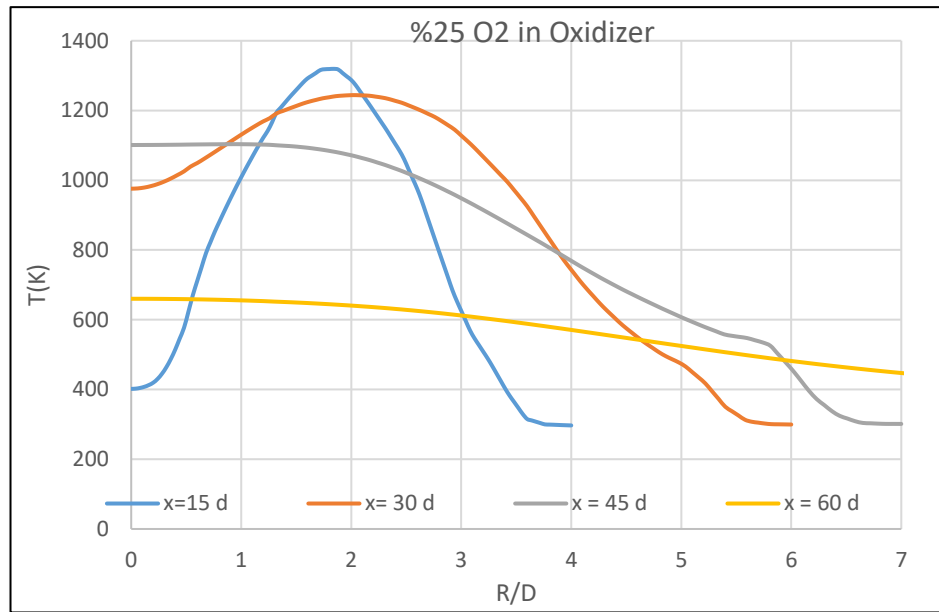


Figure 5. 28: Radial distributions of the flame temperature at various axial locations for O_2 volume fraction of 25% in the oxidizer.

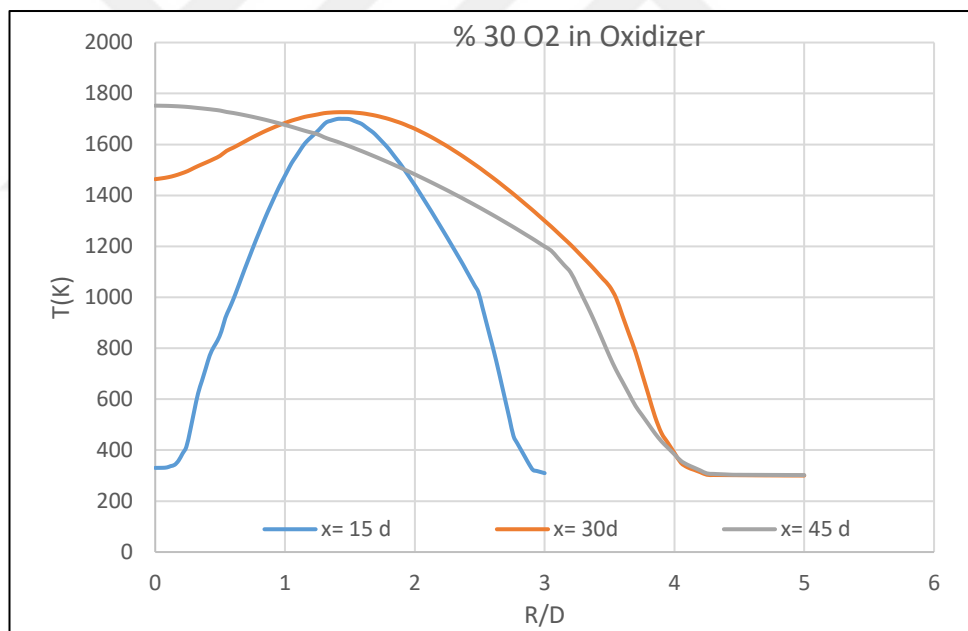


Figure 5. 29: Radial distributions of the flame temperature at various axial locations for O_2 volume fraction of 30% in the oxidizer.

For O_2 volume fraction of 25% in the oxidizer stream case, radial distributions of species mass fractions and flame temperature at various axial locations are presented in Figures 5.30, 5.31 and 5.32.

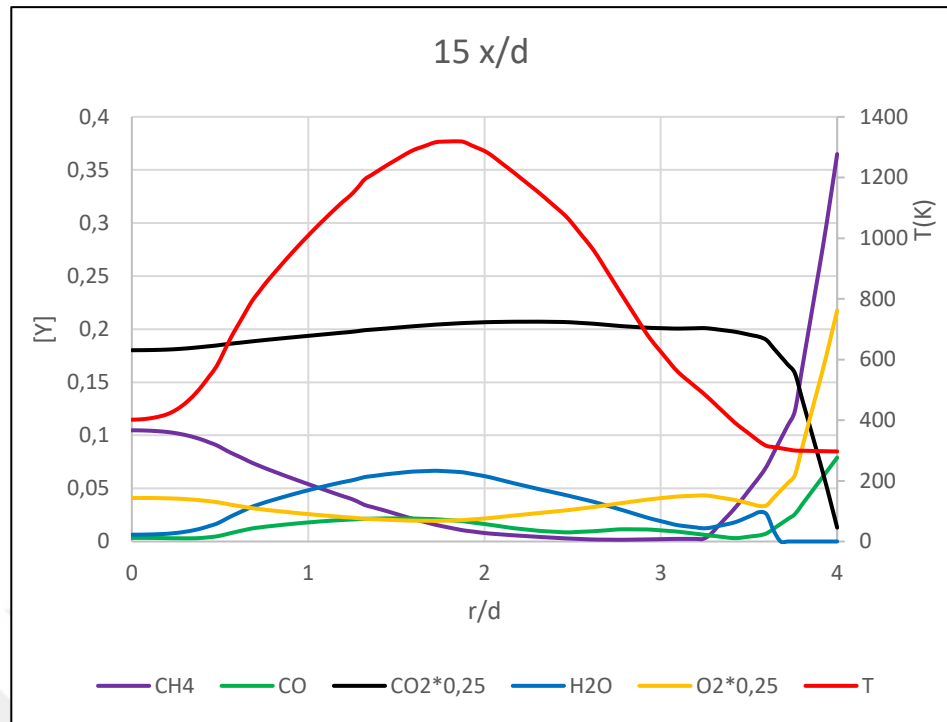


Figure 5. 30: Radial distributions of species mass fractions and the flame temperature at $x=15d$ for O_2 volume fraction of 25% in the oxidizer.

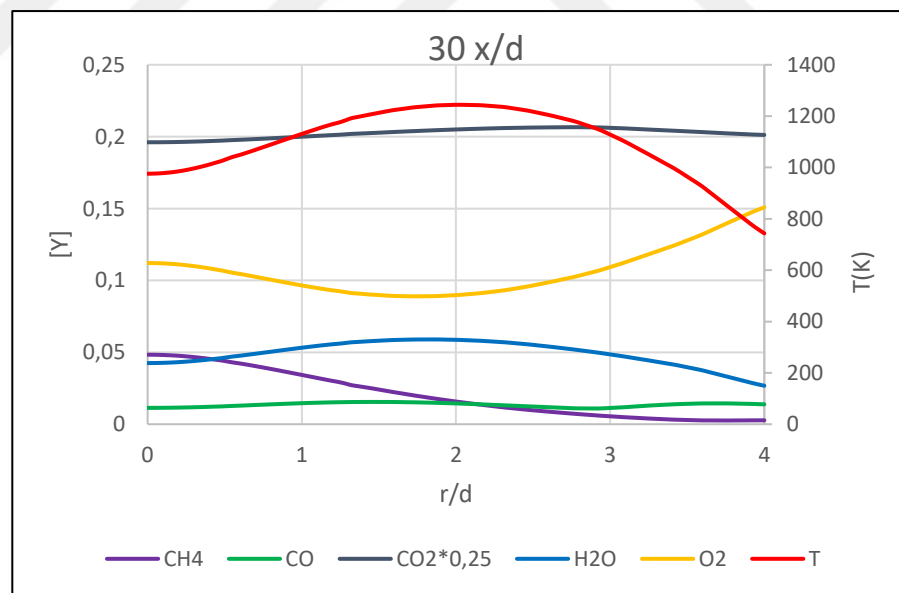


Figure 5. 31: Radial distributions of species mass fractions and the flame temperature at $x=30d$ for O_2 volume fraction of 25% in the oxidizer.

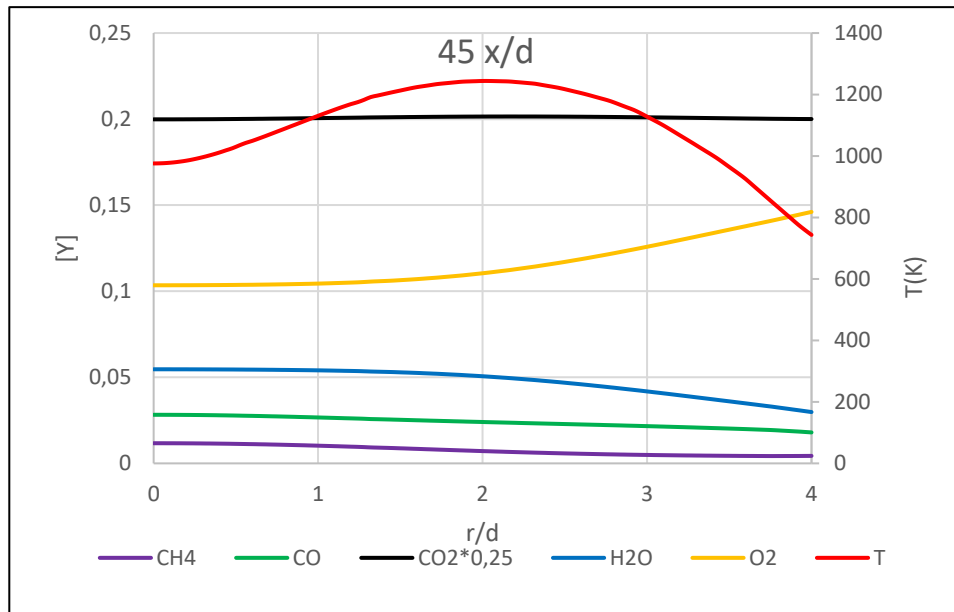


Figure 5. 32: Radial distributions of species mass fractions and the flame temperature at $x=45d$ for O_2 volume fraction of 25% in the oxidizer.

For O_2 volume fraction of 30% in the oxidizer stream case, radial distributions of species mass fractions and flame temperature at various axial locations are presented in Figures 5.33, 5.34 and 5.35.

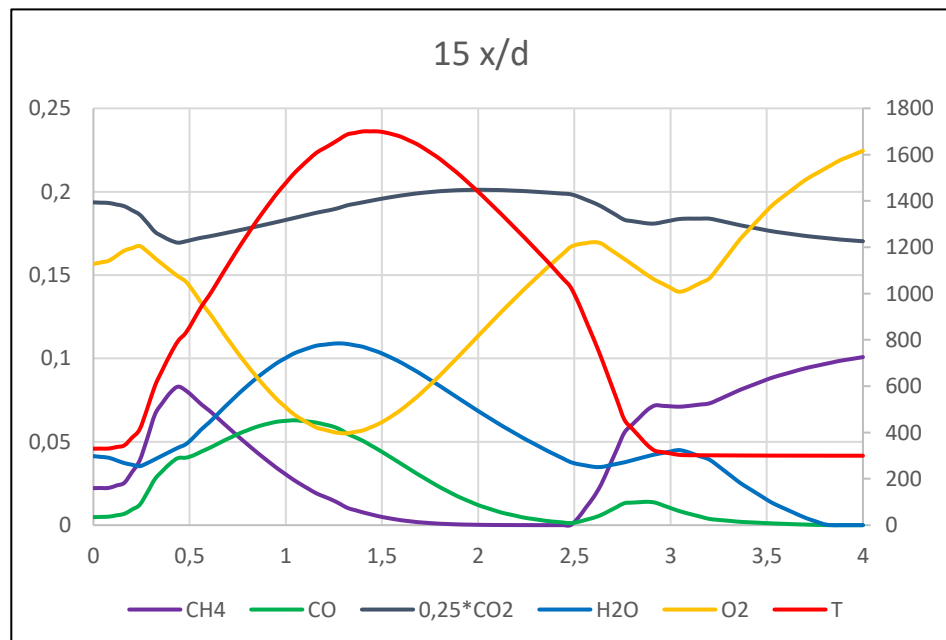


Figure 5. 33: Radial distributions of species mass fractions and the flame temperature at $x=15d$ for O_2 volume fraction of 30% in the oxidizer.

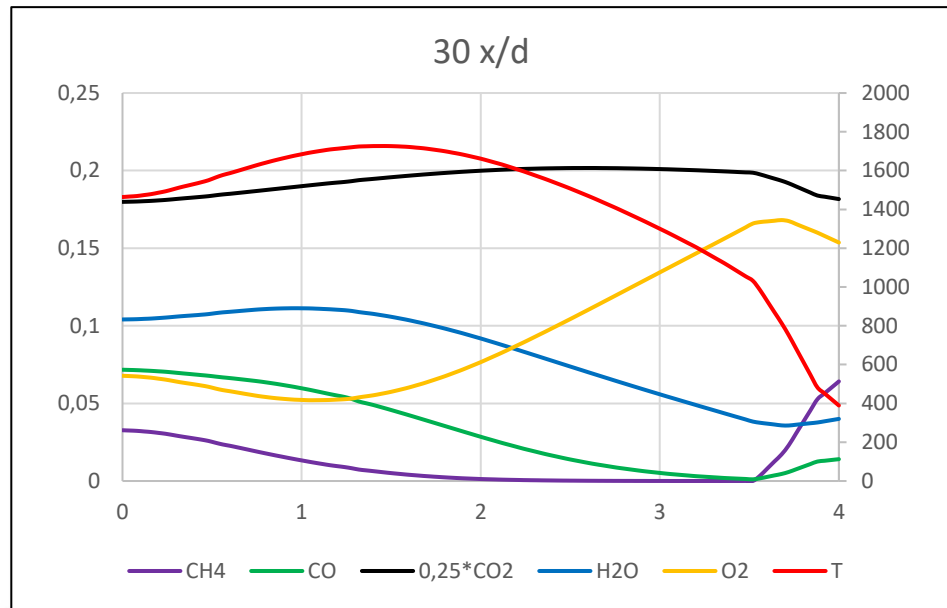


Figure 5. 34: Radial distributions of species mass fractions and the flame temperature at $x=30d$ for O_2 volume fraction of 30% in the oxidizer.

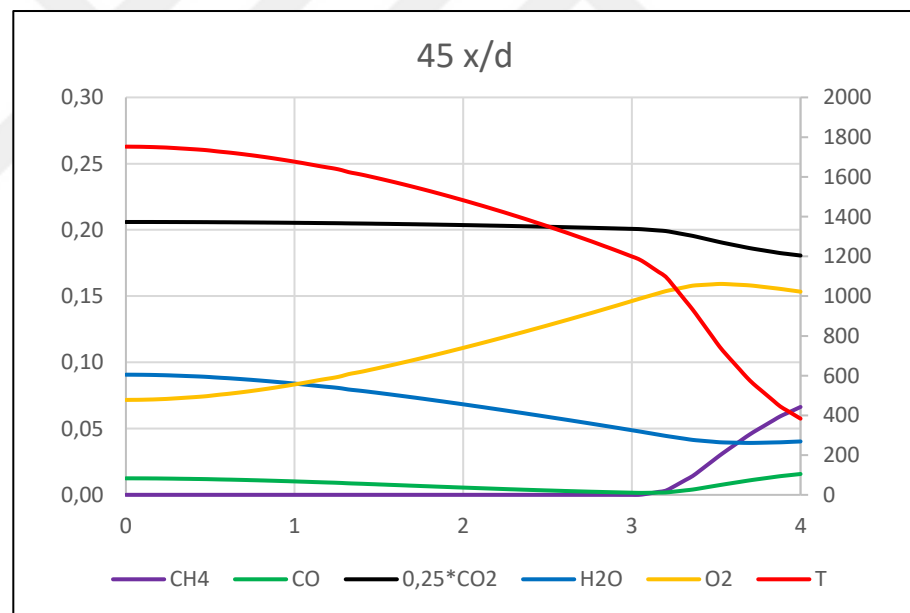


Figure 5. 35: Radial distributions of species mass fractions and the flame temperature at $x=45d$ for O_2 volume fraction of 30% in the oxidizer.

For O_2 volume fraction of 35% in the oxidizer stream case, radial distributions of species mass fractions and flame temperature at various axial locations are presented in Figures 5.36, 5.37 and 5.38.

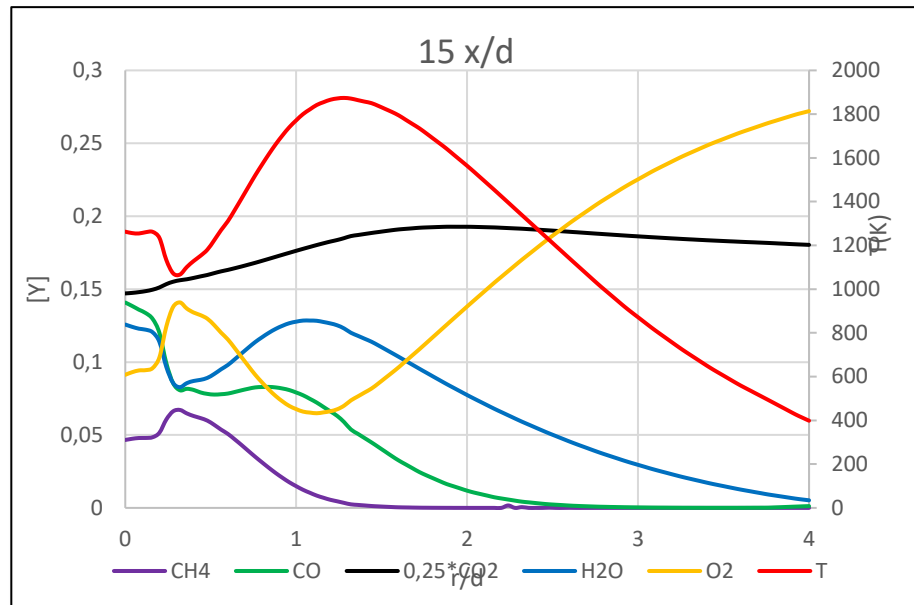


Figure 5. 36: Radial distributions of species mass fractions and the flame temperature at $x=15d$ for O_2 volume fraction of 35% in the oxidizer.

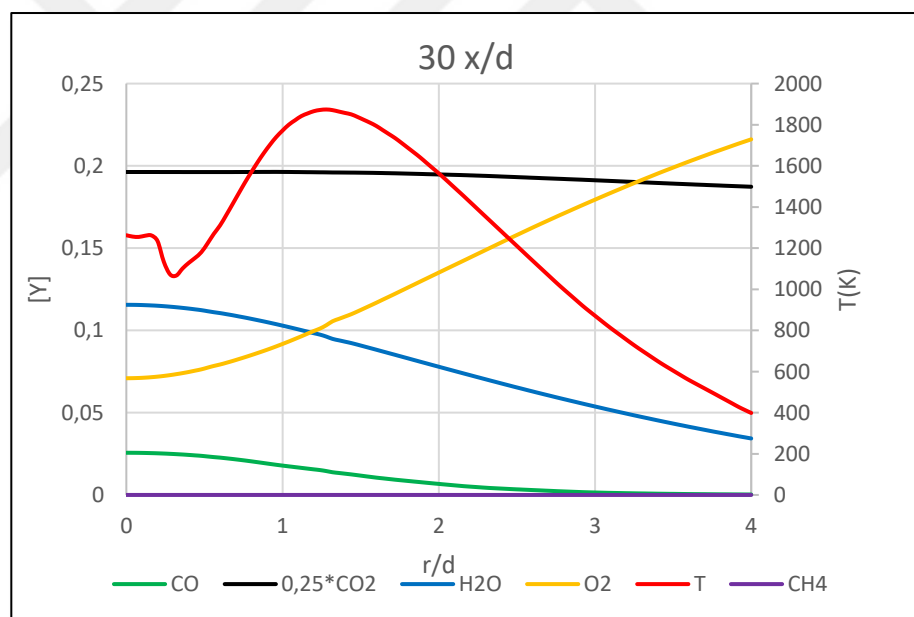


Figure 5. 37: Radial distributions of species mass fractions and the flame temperature at $x=30d$ for O_2 volume fraction of 35% in the oxidizer.

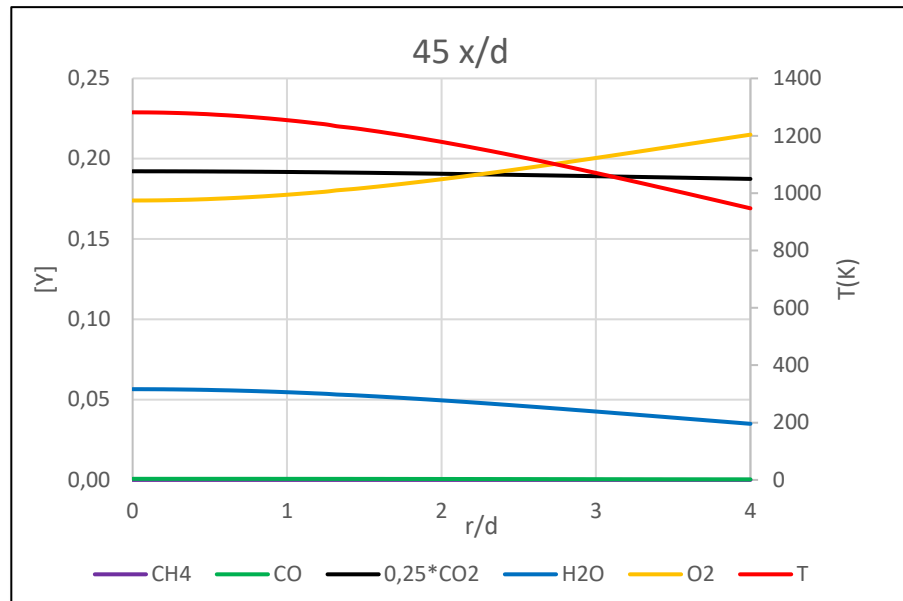


Figure 5. 38: Radial distributions of species mass fractions and the flame temperature at $x=45d$ for O_2 volume fraction of 35% in the oxidizer.

6. CONCLUSION

In this thesis turbulent diffusion combustion of a fuel mixture in oxy-fuel atmosphere at atmospheric pressure is simulated by RANS-SLFM approach for various O_2 volume fractions in the oxidizer mixture and various temperatures of the reactants. Combustible mixture consists of 25% methane (CH_4) and 75% oxidizer ($O_2 + CO_2$) by volume. In this thesis, various compositions of the oxidizer stream with O_2 volume fractions of 25%, 30% and 35% are considered in CFD simulations of turbulent oxy-fuel diffusion combustion of methane. Oxy-fuel turbulent diffusion flame characteristics are analyzed by CFD simulations for three different inlet temperatures of the reactants to the combustion chamber, namely 300 K, 500 K and 700 K, for O_2 volume fraction of 30% in the oxidizer stream case. Studied cases are simulated by computationally cost-effective Steady Laminar Flamelet Model, SLFM, under Reynold Averaged Navier Stokes, RANS, framework. RANS-SLFM approach speeds up the computations by decoupling chemistry calculations from RANS equations. Species mass fractions and enthalpies are tabulated in mixture fraction space for a variety of scalar dissipation rates. turbulence-chemistry interactions are considered by β -pdf integration. In addition to RANS equations, two more transport equations are solved for mean mixture fraction and its variance. Species mass fractions and enthalpies are looked-up from tabulated chemistry. Finite rate chemistry effects are evaluated under counter-flow diffusion flame configuration by detailed chemical kinetics mechanism GRI 3.0. Flame extinction and flammability characteristics are presented by pointed out parameters.

Changes in the temperature of the reactants and compositions of the mixture influence thermodynamic and transport properties of the gaseous mixture. Dynamic viscosity of the fuel mixture increases if both O_2 volume fraction and temperature of the reactants are increased. However, density and momentum flow rate decrease if O_2 volume fraction of the oxidizer stream and temperature of the reactants are increased for a specified inlet velocity. Changes in density and viscosity effect the Reynolds number of the fuel jet which influences the mixing behaviour of the fuel jet and the oxidizer stream. Reynolds number of the fuel mixture decreases with increased temperature of the reactants and O_2 volume fraction of the oxidizer stream. By increasing momentum flow rate of the fuel, resistance of the reaction against

aerodynamic strain effects becomes weaker. So, in the case of O_2 volume fraction of 25%, blow off occurs because of the highly CO_2 diluted oxidizer mixture. Generally, fuel jets decay in a shorter distance when momentum flow rate of the jet is decreased.

CO can be fully consumed if O_2 volume fraction of the oxidizer mixture is increased to 35%. Although fuel flammability limits are enlarged by increasing the temperature of the reactants, fuel and oxidizer streams do not mix well near the injector for the 700 K reactants' temperature case because of low Reynolds number.

Briefly, oxy-fuel diffusion flame can be anchored to the injector for 35% O_2 volume fraction in the oxidizer case. Although increased reactant temperature leads to enlarged flammability limits, 35% O_2 volume fraction in the oxidizer case can consume CO well.

Future study can focus on analyzing detailed behaviour of oxy-fuel turbulent diffusion flames by Large Eddy Simulations. CFD analyses can be improved by Flamelet Progress Variable approach which considers unsteady flame issues such as extinction and re-ignition. Furthermore, drawbacks of the flamelet model can be evaluated. If the flame interacts with a cold wall, reaction rate decreases, and high Damkohler number assumption breaks down. This drawback can be avoided by implementing frozen chemistry assumption at the wall.

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