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Modeling The Interactions Between Turbulence And Radiation In Oxy-Combustion Flames

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MODELING THE INTERACTIONS BETWEEN TURBULENCE AND RADIATION IN
OXY-COMBUSTION FLAMES

by

Md Ashiqur Rahman

BS in Mechanical Engineering, Bangladesh University of Engineering and Technology, 2007

A Thesis

Submitted to the Graduate Faculty

of the

University of North Dakota

in partial fulfillment of the requirements

for the degree of

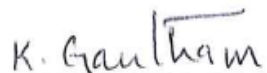
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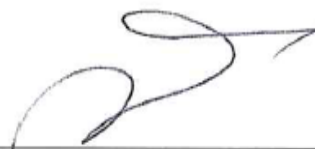
This thesis, submitted by Md Ashiqur Rahman in partial fulfillment of the requirements for the Degree of Master of Science in Chemical Engineering from the University of North Dakota, has been read by the Faculty Advisory Committee under whom the work has been done and is hereby approved.



Dr. Gautham Krishnamoorthy

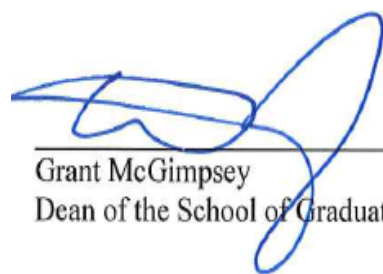


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This thesis is being submitted by the appointed advisory committee as having met all the requirements of the School of Graduate Studies at the University of North Dakota and is hereby approved.



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ABSTRACT

In order to accurately estimate radiative heat transfer in turbulent combustion systems, one needs to take into account the non-linear interactions between the temporally fluctuating species and temperature variables and the radiation field. Simply employing time-averaged values of these variables in the radiation calculations to estimate absorption and emission (as is commonly done in the modeling community) can result in gross errors in the estimation of the radiative fluxes. Therefore, models that account for these Turbulence-Radiation Interactions (TRI) have been proposed in the literature to improve the fidelity of the radiative transfer calculations. TRI models accomplish this by computing appropriate time-averaged representations of the absorption and emission terms by taking into consideration the interactions and relationships between these terms and the fluctuating species and temperature fields. However, knowledge of the specie and temperature fluctuation statistics is key to developing these TRI relationships.

In this thesis, statistical analysis of high-fidelity experimental measurements in five oxy-fuel flames with fuel jet Reynolds numbers ranging from 12,000 to 18,000 and fuel compositions in the range (50% H₂-50% CH₄ to 40% H₂-60%CH₄) were first carried out to formulate TRI models of absorption and emission. Statistical analysis of the measurements showed that in spite of the high concentrations of the radiatively participating gases in these flames, the temporal variations in the absorption field were determined to be insignificant. However, strong fluctuations in the emission field were observed and was found to correlate well with the root-mean-square of temperature.

Next, a TRI model for emission based on this experimentally observed correlation was implemented as a User-Defined Function (UDF) in the computation fluid dynamic code ANSYS

FLUENT. Time-averaged simulations of the five flames were then carried out to examine the impact of the new TRI model on the radiation field. Turbulence was modeled employing the realizable k-epsilon model and non-adiabatic mixture fraction relationships were employed to represent the chemistry. The radiative properties of the mixture were determined employing a weighted-sum-of-gray gases model developed at the University of North Dakota. The predicted temperature and CO₂ mole fractions agreed well with the experimental measurements suggesting the adequacy of our modeling procedure. The radiant fraction in these flames without accounting for the effects of TRI was 8%. However, including the TRI model predicted a radiant fraction of 16% as a result of significant enhancement in the emission term. Therefore, numerical simulations that do not adequately account for the TRI effects in these flames can significantly under-estimate the resulting wall radiative fluxes. Further, despite the absence of fluctuations in the absorption term, the magnitude of the absorption term was nearly equal to that of the emission term across all flames. This also indicates that the “optically thin” radiation approximation (which neglects absorption) that has traditionally been employed to simulate similar laboratory flames can again result in a significant over-estimation of the radiative fluxes. Finally, our preliminary calculations indicate that despite the importance of TRI models for wall radiative flux estimations, the impact of their inclusion on the flame temperature and specie field predictions was negligible.

CHAPTER I

INTRODUCTION

High Fidelity Numerical Modeling and its Necessity in Combustion Technology

Combustion processes using high fidelity numerical modeling can be used to predict temperatures, species concentrations, heat transfer, flame volume and pollutant formation that is representative of real industrial combustion systems. Models for different aspects of combustion can be added to the flow field equations to provide a full description of processes within the furnace. Different combustion procedures and flame properties are now being studied worldwide to identify promising options for power generation with efficient CO₂ capture reliability. Oxy-combustion is a promising option that is currently being considered which essentially replaces N₂ with CO₂ inside the combustor. This can significantly alter the heat transfer characteristics within the combustor due to the large differences in the thermo-physical and radiative properties of N₂ and CO₂. High fidelity computational fluid dynamics (CFD) simulations can therefore assist towards the design, operation and scale-up of these novel combustion devices. However, due to the high computational cost associated with simulating these turbulent, reacting flows (which are inherently unsteady and involve hundreds of reactions), CFD simulations are often carried out to provide a “time-averaged” representation of the turbulent flow field. This is undertaken by time-averaging the governing equations to get rid of the time dependency and “wash out” the fluctuations due to turbulence. However, a consequence of this time-averaging process is that some of the non-linear turbulent fluctuating terms do not cancel each other out and are retained after the time-averaging. Consequently, they need to be modeled appropriately. Time-averaging

of the radiative transfer equation (RTE) for instance, results in four terms (“unclosed” terms) involving medium radiative properties, temperature and radiative intensity that need to be properly modeled. However, due to the very non-linear relationships between these three variables, it is difficult to come up with simplistic “closure” models for these four terms and these are often neglected in most current CFD simulations. It has been recognized that neglecting these unclosed terms may result in 50% to 300% underestimation of the radiative fluxes from flames [1]. In this study, high fidelity laser-based measurements from oxy-combustion flames will be employed to develop simplistic models for these “unclosed” terms. This modeling strategy will henceforth be referred to in this proposal as turbulence-radiation interactions (TRI) models. It is anticipated that including the TRI into radiation modeling of turbulent flames will improve the predictions of wall heat loads, temperature field, flame structure and pollutants emission such as CO, CO₂ and NO_x.

Heat Transfer in Turbulent Combustion Flames

Accurate quantification of flame heat transfer (dominated by radiation) is important for estimating heat loads on walls of current combustor configurations, as well as assessing thermal hazards from accidental flares and fires. Turbulence in any combustion system is one of the most difficult processes to model mathematically. It involves turbulent mixing, three-dimensional fluid dynamics, radiative and convective heat transfer and very rigorous chemical kinetics. Fundamental principles and comprehensive models incorporating all of these factors are required to design the combustion systems. Since oxy-fuel technology is a promising option for CO₂ capture, an accurate estimation of heat transfer within the system is very important.

In oxy-fuel combustion, both convective and radiative heat transfer occur. However, radiative heat transfer can dominate due to the high concentrations of the radiatively participating CO₂ and H₂O gases. To calculate heat transfer by radiation it is important to solve the radiative transfer equation (RTE). In computational fluid dynamics there are several solvers that can be used. A major challenge in oxyfuel combustion is to specify the radiative properties of the gas within the furnace. Interactions of the medium with radiation occur by absorption, emission and scattering (when particles are present) that can attenuate or enhance radiation.

Necessity of Proper Radiation Modeling in Turbulent Flames

Accurate CFD simulations of industrial facilities are very important when introducing new technologies such as oxyfuel combustion. Industrial partners can use results of CFD simulations to assess furnace performance and improved design processes. This is very important when little experimental data is available. Turbulent flames are instantaneous in nature and it is very difficult to predict the spatial and temporal parameters with an average representative value. For modeling purpose to predict pollutant concentrations, accurate temperatures are critical to be determined as the chemical kinetics are dependent on the temperature. It is also computationally very expensive for the detailed treatment of radiative transfer within a turbulent flame. In order to include the effect of radiation in turbulent combustion models, without significantly increasing computational expense, a simplified treatment of radiative heat loss is needed. Model development with respect to radiative transfer will improve CFD results for oxyfuel combustion and increase confidence in computational predictions. The capability of furnace models will be improved and will provide a valuable tool for industry.

Turbulence Radiation Interaction

In reacting turbulent flow mean heat fluxes are not only influenced by the temperature and molar fractions of the species but also by the scalar fluctuations. The interactive non-linear relation between the emission and the temperature is the main cause and termed as interaction between turbulence and radiation. The interactive effect of radiation and turbulence on the flow field of these turbulent flames has been recognized through experimental, theoretical and computational manner. It has been recognized by these studies that considering the turbulence radiation interaction is very important when the turbulence fluctuation and radiative source terms are much higher and radiative emission becomes important. So better modeling of thermal radiation taking turbulence fluctuations into account becomes important too. Becker [2] from his experimental and theoretical study established the local root mean square (rms) of volumetric radiative energy emitted by the flame along the centerline varied between 20% and 500% of the mean value at the same location. Cox [3] studied the influence of turbulence on the emitted radiative heat transfer by a hot medium. These experimental data confirmed theoretical results that shows the variation of the emission radiative transfer from the mean which is significant. Coelho [4] studied a turbulent diffusion flame showing the turbulent fluctuations contributing to reduce the mean absorption co-efficient of the medium increased by turbulence. His theoretical study also revealed that turbulence effects are more pronounced at highly fuel-rich or fuel-lean conditions than in stoichiometric conditions.

Different Simulation Procedures

RANS or Reynold's Average Navier-Stokes equation is the most widely used one where we take the mean value of the total flow field temporally. Different models like k- ϵ , k- ω ,

Reynold's Stress Model are used according to best practice. The RANS model is based on conserved scalar/prescribed pdf or transport pdf methods to account TRI. In the conserved scalar/prescribed pdf method, the conserved scalar is generally taken as the mixture fraction, and transport equations are solved for the mean and the variance of mixture fraction. These two quantities are sufficient for the definition of the pdf of mixture fraction, which is assumed to be either a beta function or a clipped Gaussian [Coelho, 2012]. The mean flow properties (mass fractions, temperature, and density) are determined from integration of the instantaneous values, expressed as a function of mixture fraction and scalar dissipation rate, weighted by the pdf of mixture fraction, over the mixture fraction range. In transport pdf based methods the transport equation for a joint pdf are addressed. This joint pdf is derived from the transport equations of the dependent variables and may include the velocity, temperature, and species concentration fields or just the composition (temperature and species concentration) field. No assumption about the shape of the pdf is needed. The main advantage of these models is that the chemical source terms are treated exactly, without any modeling assumptions. However, models are needed for molecular mixing, pressure fluctuations, and viscous dissipation effects.

Direct numerical simulation (DNS) is another approach which does not consider the time averaged conditions. The complete time history of the velocity is calculated at a micro-scale level named Kolmogorov microscale [Turns, 2012]. At this scale level the molecular effects are significant. This needs huge computational requirements for these complex turbulent combustion systems but it provides fundamental and reliable insight into the physics of turbulent flows and it can be used to investigate turbulence radiation interaction.

LES or large eddy simulation is an approach that combines attributes of both DNS and statistical turbulence modeling methods [Turns, 2012]. It resolves the flow scale to much larger

than the microscale level but models the turbulence at scales smaller than the previous ones mentioned. Basically large scales of motion which are energy-containing are explicitly computed but not modeled [Turns, 2012]. Therefore this contains the true physics of the flow. This is very much applicable for the combustion type complex reaction models.

For our research purpose we will be using the RANS model with a turbulence radiation interaction model for emission based on the experimentally observed correlation which was implemented as a User-Defined Function (UDF) in the computation fluid dynamic code ANSYS FLUENT. Time-averaged simulations of the five flames were then carried out to examine the impact of the new TRI model on the radiation field. Turbulence was modeled employing the realizable k-epsilon model and non-adiabatic mixture fraction relationships were employed to represent the chemistry.

Including the Data Analysis Results for Turbulence in RANS Modeling

DNS and LES being computationally expensive the goal of this research was to use the time-averaged RANS modeling with commercial code ANSYS FLUENT with and improvement and added user defined functions (UDF) to recognize the turbulence radiation interaction. To recognize the interaction of temperature and emission radiation interaction the laser based data from the experiment around the lower region of the flame were statistically analyzed and the variances on each data point for temperature and chemical species were determined. The fluctuation or deviations from mean data were then calculated. Temperature self-correlation data were $\frac{\overline{T^4}}{\overline{T}^4}$ plotted against the temperature fluctuation intensity $\frac{\overline{T'^2}}{\overline{T}^2}$. Strong fluctuations in the emission field were observed and was found to correlate well with the temperature fluctuation intensity. Statistical analysis of the measurements showed that in spite of the high concentrations

of the radiatively participating gases in these flames, the temporal variations in the absorption field were determined to be almost insignificant.

CHAPTER II

THEORETICAL BACKGROUND

Oxy-fuel Combustion Technology

Oxy-combustion technology is the focal topic of this paper. So, we go into details into this technology through the figure 1 below.

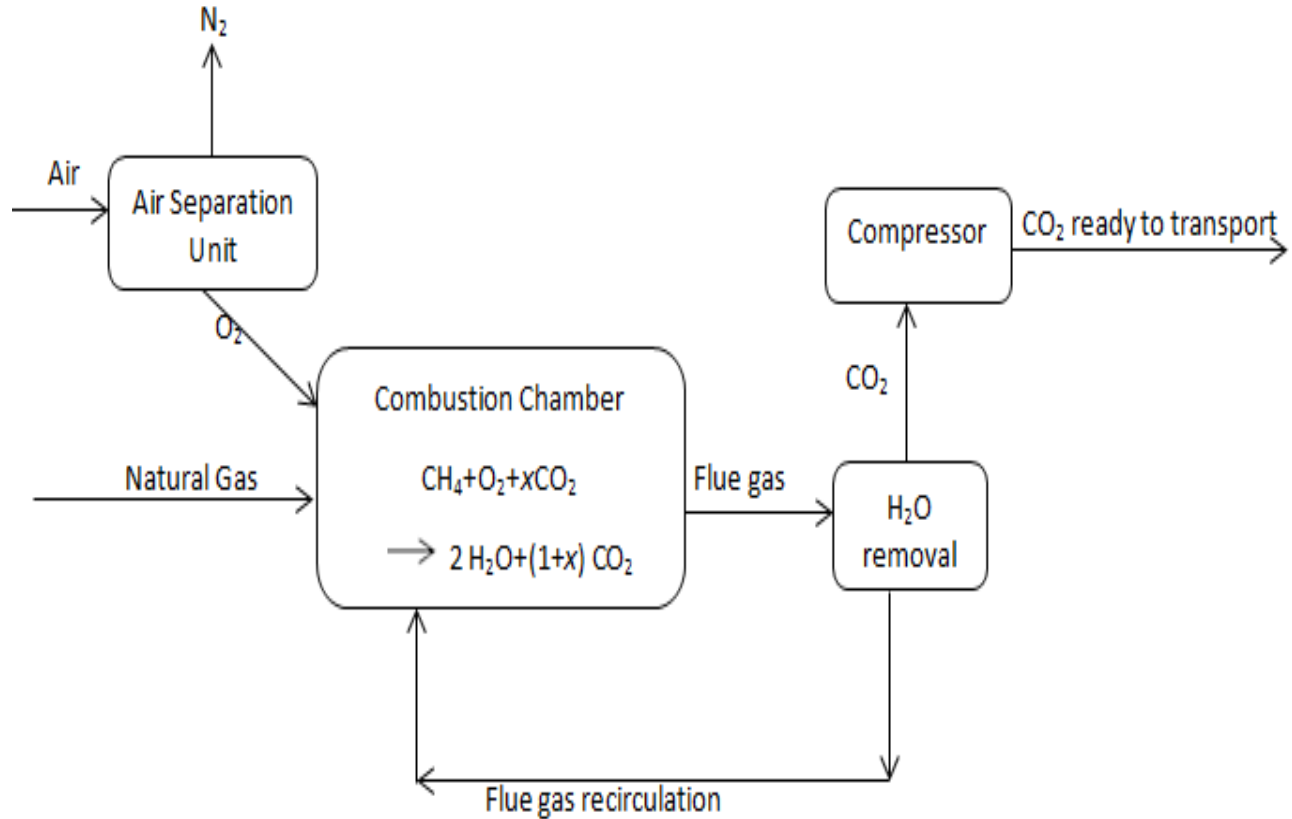


Figure 1: Schematic of oxy-combustion technology using CH₄ as fuel, Adapted from [Sevault, 2012]

Starting with the air separation unit (ASU) which separates out the O₂ from incoming air. O₂ is the main component for the oxidation process of the fuel that is going to be burnt. The O₂ is then

carried to the combustion chamber where it burns with the fuel. The flue gas of the oxy-fuel combustion system is a combination of CO₂ and H₂O gas. By condensing the flue gas mixture the H₂O stream can be separated out from the product of the combustion chamber. Part of the flue gas is also recirculated back again. As there is no nitrogen gas coming in we do not need to worry about NO_x formations in the flue gas though in reality some percentage of nitrogen do come in as the efficiency of the air separation unit can't be 100%. Neglecting the fact that NO_x formation and other gas formation still might occur we can assume a relatively pure CO₂ stream from the system. High concentrations of CO₂ may affect several aspects of combustion including turbulence, heat transfer and chemistry due to the different properties of the gas compared to nitrogen. The flue gas recirculation is a part of the CO₂ stream which is sent back to the combustion chamber, while the rest is compressed for transport for CO₂ storage. Depending on the purity of the fuel and the oxygen supply, a supplementary separate purification stage may be required to filter out some unwelcomed gas stream, such as oxygen, argon, nitrogen, sulfur oxides or nitric oxides, for instance. The main purpose of this oxy-fuel system is to use the heat of combustion to generate steam and run a turbine. Another configuration of interest while firing natural gas is to use the products of combustion directly as a working fluid in a turbine. It is evident from the discussion that, combustion under oxy-fuel conditions is fundamentally different at intake and at the product side from air-fired combustion. This presents new challenges such as the combustion fundamentals, burner conditions, air to oxygen production, flue gas treatment and recirculation, process thermal integration and optimization. In the past decade, a lot of efforts have been made in this area.

Advantages

Oxy-combustion technology using flue gas recirculation compared to other combustion technologies has some advantages. One of them is wide temperature variability for operating condition control which is very useful for different test purpose. Comparatively pure CO₂ stream than the other technologies is another important factor. Oxy-fuel boilers can be retrofitted on the existing plant with recirculation which decreases the flue gas volume compared to air—fired plants. These types of plants have great potential to reduce emissions of pollutants like NO_x, SO_x, particulate matters. So we can see that there are some very important technological aspects such as reliability, heat efficiency, flue gas re-usability which impact the combustion system.

Limitations

The level of oxygen purity is the main concern for the air separation units. The units are very energy consuming and need to be in large scale. The energy consumption increases with the level of the purity of the oxygen stream. It takes more than half the power of the oxy-combustion process and we need to trade-off the amount of purity needed against the power of consumption with products we get and control the pollutant capture so that the overall efficiency is best achieved.

Non-Premixed Oxy-Combustion Flames

Non-premixed flames are much safer than the premixed flames as fuel and oxidizer keep separated up to the reaction zone. In non-premixed flames, there are two streams of fuel and oxidizer which are separated and these two streams come to meet at the reaction zone. The diffusion mechanism mixed with the turbulent nature of the reactants going inward direction and

products going outward direction of the reaction zone help the fuel to burn. Turbulent nature of the flame dominates the reaction rates and molecular transport by turbulent mixing. The total energy changes from the reactants to the product creates stoichiometric conditions producing maximum possible flame temperature.

Non-premixed jet flames depending upon the velocity of the nozzle output can be divided into three different regimes: laminar, transitional and turbulent jet flames. A non-dimensional number is generally used to determine the regime followed by a jet flame. This non-dimensional number is termed as Reynold’s number (Re_f) which basically is a function of velocity of the fuel stream for a certain burner and combustion system

$$Re_f = \frac{Vd}{\nu} \dots\dots\dots(1)$$

Where V= mean velocity of the fuel nozzle outlet (ms^{-1})

d= diameter of the fuel nozzle (m)

ν = kinematic viscosity (m^2s^{-1})

Figure 2 adapted from [Hottel 1949] gives a clear picture of the gradual changes from the laminar to turbulent nature of the flame with an increasing jet Reynolds number. The jet flame is laminar when the value of the Reynolds number for it is below 1000. It is then dominated by molecular diffusion. Its flame length increases continuously with the jet Reynolds number. When Reynold’s number reaches the value of 1000 – 2000, the flame enters the transitional region. The flame length here decreases with Re_f . When the value of the Reynold’s number of the jet flame becomes 3000 it enters into the turbulent regime and it is fully developed turbulent at the value of 4000. The flame length of fully developed turbulent jet flames increases till a certain range but after increasing the Reynold’s number the flame length does not vary.

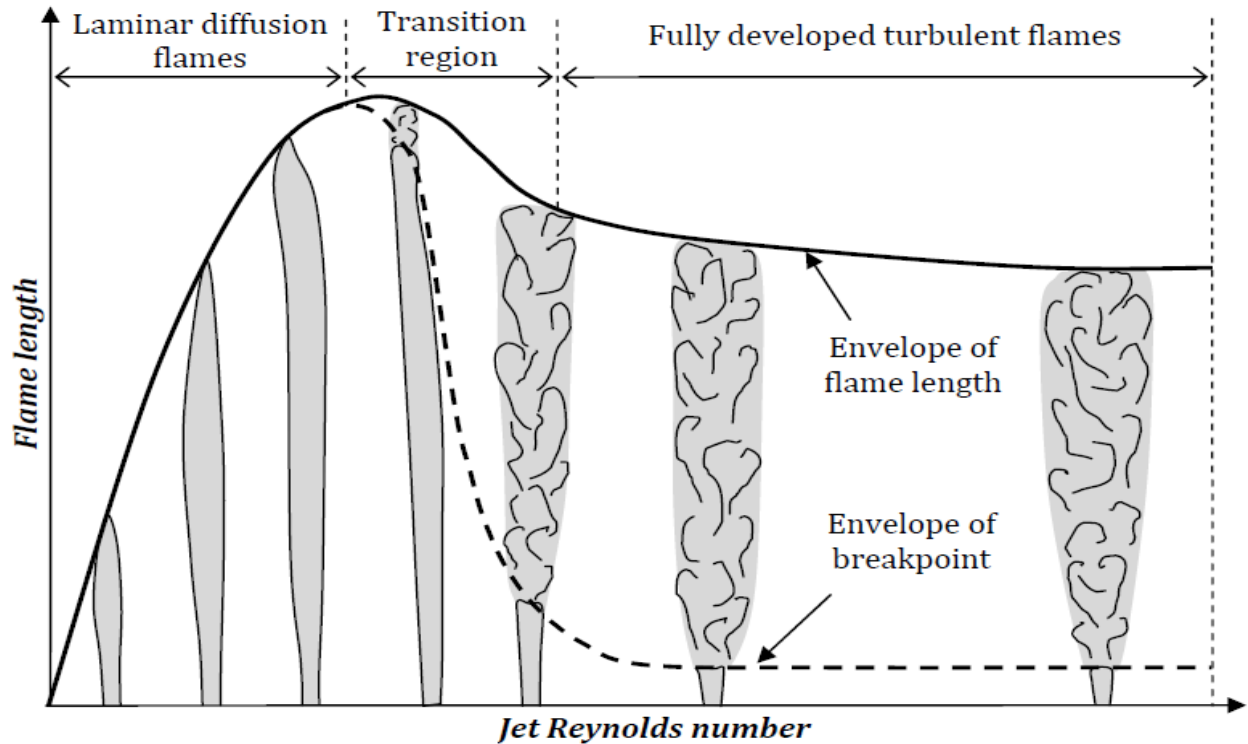


Figure 2: Schematic of the progressive change in flame regime with an increasing jet Reynolds number. Adapted from [Hottel 1949].

Radiative Transport Equation (RTE) in Combustion Flames

The radiative transfer equation (RTE) is a mathematical statement of the conservation principle applied to a pencil of radiation (ray) traveling along a path through a medium. Radiation or energy rays travelling along a path is attenuated by absorption and scattering (out scattering), and is enhanced by emission. It is a mixed form of integral and differential equation and an exact solution may only be obtained after simplifying assumptions such as uniform radiative properties of the medium, non-scattering conditions and homogeneous boundary conditions. Radiative transport equation is one of the main source of energy contributing to the change of energy in the combustion system modeling. Turbulent non-premixed flames being highly radiative in nature, the radiative transport equation plays a very important role for modeling these systems such as

gas-fired furnaces and boilers and other important industrial processes. Accurate calculation of radiative transfer is then of crucial importance for the prediction of the thermal performance. In addition, radiation significantly affects the temperature and specie field and consequently has a strong impact on the predicted formation of pollutants. However accurate quantification of the amount of radiative transfer is a very complex procedure in modeling the systems. Because radiation is extremely strong spectral dependence of the radiative properties of the combustion products. In natural gas fired combustion systems the dominant radiating species are CO₂ and H₂O. The effects of CH₄ and CO are usually highly localized in the near burner regions and thus of minor significance. Recently new methods such as weighted sum of grey gas (WSGGM) etc are developed for handling the spectral structure of the radiative properties of gases. The radiative transfer equation where the combustion products do not scatter light can be written as:

$$\frac{dI}{ds} = k \left(\frac{\sigma T^4}{\pi} - I \right) = kI_b - kI \quad \dots\dots\dots(2)$$

Where k is the absorption co-efficient, $\frac{\sigma T^4}{\pi} = I_b$ term indicates the Planck function/blackbody radiation which is the function of temperature also known as radiative emission term and I indicates the spectral radiative intensity also known as radiative absorption term.

Radiative heat transfer is dependent on the temporal temperature distribution as well as the temporal concentration field of the absorbing and emitting medium. The exact solutions for the RTE are not practical for engineering applications because these systems are multidimensional, radiative properties being spectral in nature and the medium might not be homogeneous. Also the evaluation of all the coefficients in the RTE which depend on wavelength, gas composition, temperature, pressure, type of particles, etc. is very rigorous. So using capable models for simplifying the complex differential radiative transfer equation and solving it to predict the

radiation properties of the combustion products with a similar accuracy is an important step for modeling over all heat transfer of the complex combustion systems.

Introduction to Turbulence Radiation Interaction and Temperature Self-Correlation

Many theoretical, computational and experimental analysis shows that the mean heat fluxes in turbulent combustion systems are influenced not only by the temperature and molar fraction of the species but also by the fluctuations in these variables due to turbulence. It has been recognized that the radiative heat fluxes in turbulent flows in comparison with the laminar flows may exceed more than 100% for some flames [4]. The turbulent fluctuation creates nonlinear relation between radiation, temperature and species concentration. It is very important to consider this. The radiative heat transfer equation influences the temperature and density fields. This is represented by Figure 3 below. The flow and species concentration fields are influenced by radiation because the density field in turn affects velocity field. This influences the

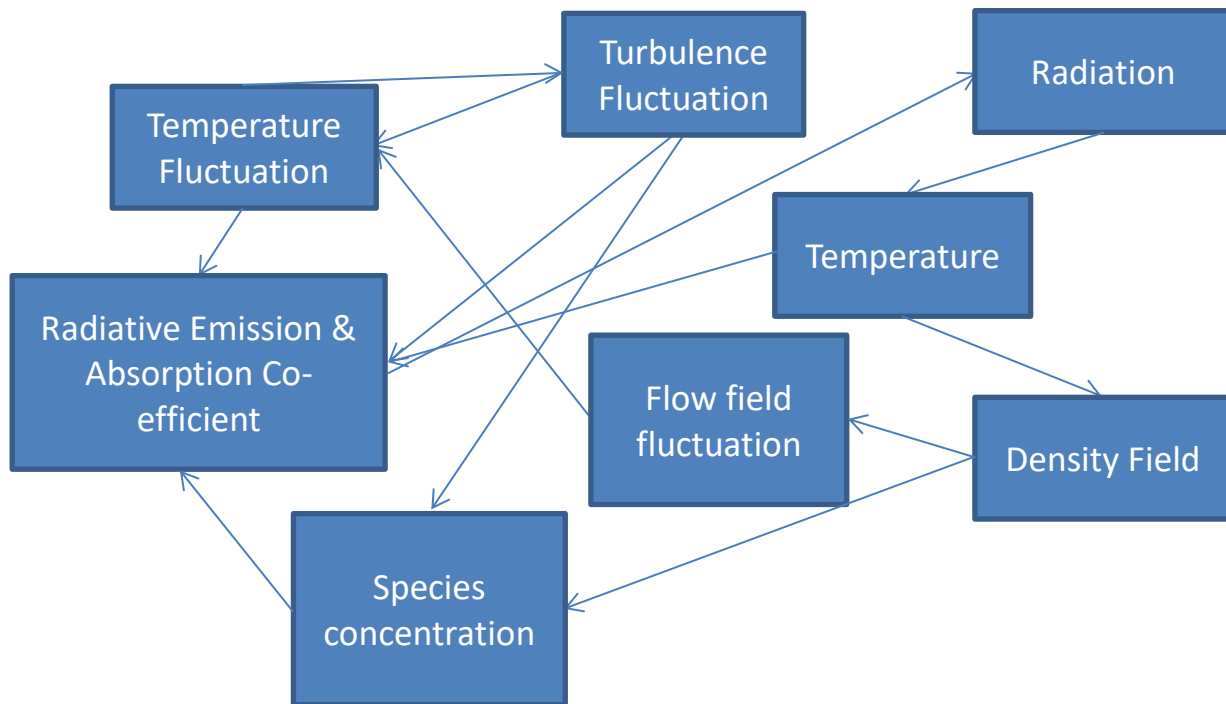


Figure 3: The role of turbulent fluctuations in coupled reactive fluid flow/radiative transfer calculations

scalar fluctuations. On the other hand density field is directly related to radiative heat transfer as radiation influences temperature and temperature affects the density. A theoretical analysis presented in [9] couples radiative transfer, thermal conduction and velocity fluctuations in post combustion gases, and shows that turbulence fluctuations of any magnitude induce radiative flux and velocity fluctuations. It has also been shown that radiation in a turbulent flow influences the temperature fluctuations and modifies the structure of the spectrum of the temperature variance [8]. Therefore, radiation influences turbulence. On the other hand, in reactive flows, the turbulent fluctuations also impact the fluctuation of temperature and specie field. These influence the radiation field, because the emission of radiation and the radiative heat flux are non-linear functions of the temperature and species concentration. The radiative properties of the medium such as the absorption co-efficient also depend on the temperature and species concentration and is influenced by the turbulence fluctuations. Thus, turbulence influences the radiation inside the flame and vice versa leading to turbulence radiation interaction terms that are very difficult to model in any turbulent combustion flames. The relations between these quantities are illustrated in Fig. 3. The absorption co-efficient depends upon the specie concentration of the temperature field, the Planck function depends upon the temperature. These three terms each consisting of a mean term and a fluctuating term for each position for the turbulence characteristics. In RANS simulation, we find the correlation between the absorption coefficient and Planck function $\overline{kI_b}$ and the correlation between the absorption coefficient and radiative intensity \overline{kI} . Researchers in the field of radiation-turbulence interaction have assumed that the correlation between the fluctuating absorption coefficient, and the fluctuating radiative intensity is negligible thus bringing down to the fact that the radiative transport equation for turbulent cases depends upon the fluctuation of the absorption co-efficient and the Planck function justified by Modest [5].

We know that the radiation energy emitted in a unit area is equal to $\epsilon\sigma T^4$. Here ϵ , is termed as emissivity which is a property of a certain medium and σ is Stefan-Boltzmann constant. It is defined as the ratio of the amount of energy emitted by the gaseous layer to the amount that would be emitted by a blackbody at the same temperature. Expressing the instantaneous temperature, T, and the emissivity, ϵ , as a sum of the mean value plus a fluctuation would yield after Taylor series expansion as (σ being a constant we can neglect it from bearing a fluctuation):

$$\overline{\epsilon T^4} = (\overline{\epsilon} + \overline{\epsilon'}) (\overline{T} + T')^4 = \overline{\epsilon} \overline{T}^4 \left(1 + 6 \frac{\overline{T'^2}}{\overline{T}^2} + 4 \frac{\overline{T'^3}}{\overline{T}^3} + \frac{\overline{T'^4}}{\overline{T}^4} + 4 \frac{\overline{\epsilon' T'}}{\overline{\epsilon} \overline{T}} + 6 \frac{\overline{\epsilon' T'^2}}{\overline{\epsilon} \overline{T}^2} + 4 \frac{\overline{\epsilon' T'^3}}{\overline{\epsilon} \overline{T}^3} + \frac{\overline{\epsilon' T'^4}}{\overline{\epsilon} \overline{T}^4} \right) \dots \dots (3)$$

The first four terms inside the parenthesis on the right side of above equation provides us with a relation of fluctuating temperature terms to the mean terms called as the temperature self-correlation, while the last four terms represent the fluctuating emissivity-temperature to the mean of the same which is termed as emissivity-temperature correlation. For gray radiative transport i.e if the emissivity or fluctuations of emissivity is neglected (cross-correlation between the temperature and emissivity is neglected) the term becomes:

$$\frac{\overline{T^4}}{\overline{T}^4} = 1 + 6 \frac{\overline{T'^2}}{\overline{T}^2} + 4 \frac{\overline{T'^3}}{\overline{T}^3} + \frac{\overline{T'^4}}{\overline{T}^4} \text{ (Temperature self-correlation equation) } \dots \dots \dots (4)$$

If we neglect the higher order terms (to be value of ≈ 0) in the temperature self-correlation equation we get:

$$\frac{\overline{T^4}}{\overline{T}^4} = 1 + 6 \frac{\overline{T'^2}}{\overline{T}^2} \dots \dots \dots (5)$$

The term $\frac{\overline{T'^2}}{\overline{T}^2}$ is defined as temperature fluctuation intensity. It indicates the fluctuation intensity i.e root mean squared value of temperature with respect to the average temperature squared.

From this straight-line equation ($\frac{\overline{T^4}}{\overline{T}^4} \text{ vs } \frac{\overline{T'^2}}{\overline{T}^2}$) the value of slope of the equation is around 6 for turbulent flames. Cox [3] through his research found out that in turbulent combustion flames the

temperature fluctuations will dominate the mean temperature effects when the temperature fluctuation intensity exceeds approximately 40%. Kabashnikov and Kmit [15] analyzed the combined effects of fluctuating absorption coefficient and temperature on radiation assuming a linear variation of the absorption coefficient with temperature on the spectral region where the influence of fluctuations is large due to the strong dependence of the Planck function on the temperature.

Radiant Fraction

Radiant fraction is an important term used to compare the amount of radiation energy released with respect to the total heat energy from the combustion. It can be written as the ratio of the radiation heat energy transferred from the flame to the surrounding area and the total heat of combustion. The following equation represents the radiant fraction:

$$\chi_R \equiv \frac{\dot{Q}_{rad}}{\dot{m}_F \Delta h_c} \dots\dots\dots (6)$$

where \dot{m}_F is the mass flow rate of fuel supplied to the flame and Δh_c is the fuel heat of combustion. Depending on the fuel type and flow conditions, radiant fractions for jet flames range from a few percent to more than 50 percent [Turns, 2012].

There are two sources of radiation in flames: molecular radiation, primarily from molecules like CO₂ and H₂O; and essentially from the blackbody radiation from in-flame soot. Normally methane flames contain very little in-flame soot [Turns, 2012] corresponding to the molecular radiation dominance. In our study, we will be using the methane/hydrogen flames in order that we can take care of in-flame soot radiation and can only consider the molecular radiation characteristics.

CHAPTER III

METHODS

Experimental Set-Up

The experimental set-up was done by Dr. Alexis Sevault as a part of his research work at Sandia National Lab. the main burner is a co-flow and the inside diameter is 96.5 mm, with a 5 mm inside diameter central nozzle for fuel. The oxidizer mixture ($O_2/C O_2$) is issued by the co-flow, while the fuel mixture (CH_4/H_2) flows through the central nozzle. Perforated plates and a honeycomb are mounted inside the co-flow to allow a uniform flow distribution of the oxidizer. The fuel nozzle has 0.5 mm wall thickness and squared off end to help stabilize the jet flames.

Its tip is 40 mm above the co-flow and is long enough, so that the flow is considered fully developed and fully mixed when the fuel mixture reaches the nozzle tip. The burner is mounted at the top of a 25 cm x 25 cm square section wind tunnel from where fresh air flows at 0.5 m/s to accompany the flow and to prevent from early mixing with ambient air. This enables to confidently perform measurements in the near field of the axisymmetric jet flames, from 1 to 20 diameters above the nozzle, without requiring confinement in a combustion chamber. Figure 4 shows the CAD drawing of the burner. Measurements were performed using the simultaneous line imaging of Raman/Rayleigh scattering (LRS) in non-premixed $CH_4/H_2 - O_2/CO_2$ jet flames in a co-flow burner. The measurements could not be performed without mixing H_2 in the stream due to the high level of soot, so that hydrogen dilution of the fuel was considered. Due to H_2

mixing the flame remained attached to the fuel nozzle. Two series of three flames have been performed: one with varying the jet Reynolds number from 12,000 to 18,000, and another with

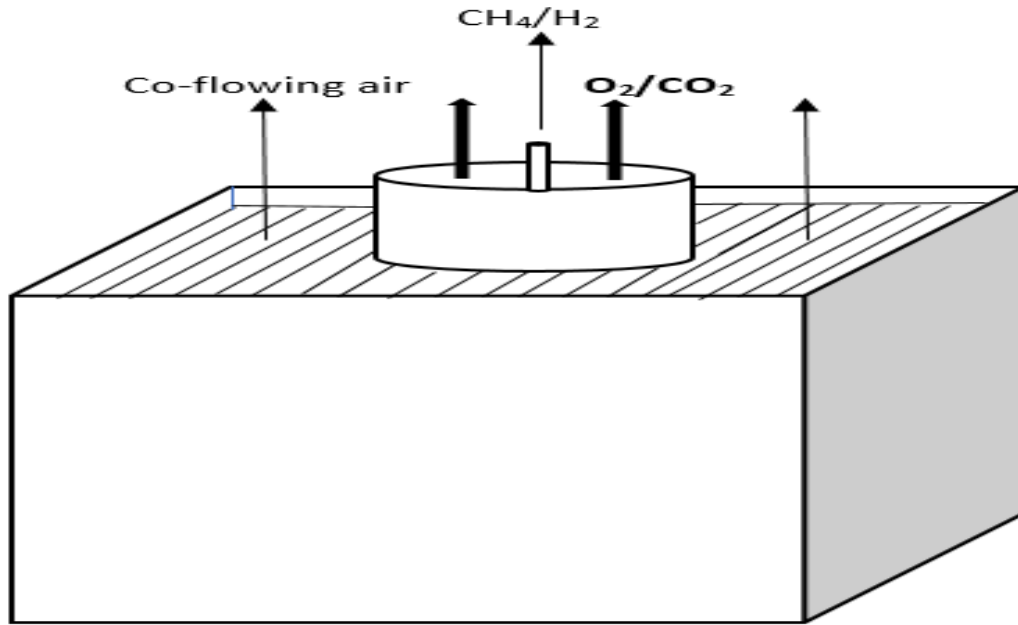


Figure 4: CAD drawing of the co-flow burner used for CO₂ diluted oxy-fuel jet flames measurements at SNL; (Sevault Dissertation, 2012)

varying the hydrogen dilution in fuel from 37 to 55 %mol. Flames conditions are given in Table

1. The oxidizer is composed of 32 %mol O₂ in the oxidizer and the flames have been generated

Flame		%mol O ₂ in Oxidizer	%mol H ₂ in Fuel	Reynold's Number, Ref	Jet Speed (m/s)	Co-flow speed (m/s)	Tad (K)
Experiment name	Designated in the simulation as						
A-1	A	32	55	15000	98.2	0.778	2250
A-2	B	32	45	15000	84.4	0.755	2243
A-3	C	32	37	15000	75.8	0.739	2236
B-1	D	32	55	12000	78.6	0.622	2250
B-2	A	32	55	15000	98.2	0.778	2250
B-3	E	32	55	18000	117.8	0.933	2250

Table 1: Experimental Flame Conditions and designated flames used in the simulation

LRS setup has enabled to achieve results of great quality for the main species concentrations and the temperature.

CFD Modeling

Geometry and Mesh

The domain was modeled in a 2D axisymmetric modeling as shown in figure 5 where the fuel burner, co-flow burner and the air inlet is shown with an extended domain at the top which is open to atmosphere (atmospheric pressure). The entire geometry was meshed employing three different control volume for meshing convenience and the ease of simulation run time and the results of the variables reported in this study were found to be varying. The CFD simulations were carried out using the commercial code ANSYS FLUENT [19]. The pressure velocity coupling method was the SIMPLE algorithm in ANSYS FLUENT [19] solution which we have determined from past experience to perform well in such conditions. The standard and 2nd order upwind schemes were employed for the spatial discretization of the pressure and momentum terms respectively. Steady state simulations were run. To model the radiative heat loss it needs the radiative transfer equation (RTE) to be solved to calculate the radiative source term for the energy equation solving through RANS averaging. The calculation of radiative heat losses in turbulent flames has classically been based on the ‘optically thin’ approximation, thus neglecting flame absorption, particularly in the case of non-luminous flames [15]. In this work, several different closures (TRI models) are considered and the strength of the effect of fluctuations in the non-linear temperature factor in the emission term and the importance of fluctuations in the absorption and emission coefficient are investigated.

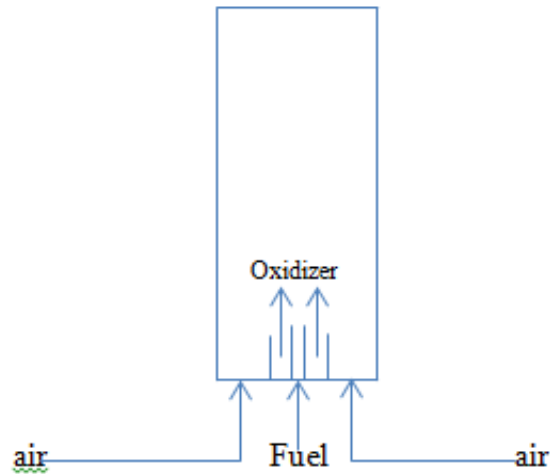


Figure 5: 2D Axi-symmetric model of the simulation field

Radiation Modeling

The radiation was modeled by solving the radiative transport equation (RTE) employing the discrete ordinate (DO) model. Yin [12] in the semi industrial furnace used the DO radiation model with revised WSGGM model. Wheaton et al [13] in their 0.8 MW turbulent model also used the DO radiation with revised WSGGM model. Using this radiation model both were able to better predict the temperature and species concentration specially CO concentration downstream of the furnace. The angular discretization was carried out by employing a 3×3 theta \times phi discretization. The adequacy of this angular resolution was established by ANSYS FLUENT user's guide [10] for angular direction with any further increase in angular resolution. The radiative properties of the gas mixtures were all determined employing a recently proposed WSGG model [20]. This model with five gray gases, developed at University of North Dakota, accurately calculates the radiative properties of CO₂ and H₂O vapor mixtures in the combustion systems consisting methane, natural gas, or coal as fuel which are combusted in air-fired and oxy-fired conditions.

Chemistry Modeling:

The gas-phase chemistry modeling is the hardest job in properly modeling the combustion systems. The gas-phase chemistry was modeled by using the equilibrium probability density function (PDF) based mixture fraction model which has non-adiabatic extensions. For the PDF table chemical equilibrium state relation was used with non-adiabatic energy treatment because of the multiple streams (fuel, O₂/CO₂ and air flow) were modeled. In a previous study Abdul Sater and Krishnamoorthy [18] studied the appropriateness of employing the non-adiabatic formulation of the equilibrium PDF based mixture-fraction model (denoted as PDF) for these types of turbulent flames and the flame length and temperature predictions were found to agree well with the experimental measurements. Wheaton et al [13] also in his 0.8 MW turbulent model used the non-adiabatic equilibrium form of PDF and found good agreement for temperature prediction and experimental measurement. Mixture fraction is normally used in the systems where the fuel and oxidizer streams are separate and their instantaneous thermochemical state is related to its mixture fraction and its enthalpy. The benefits of this model is that it becomes a single and source less conservation equation for the all the species mixture fraction due to the reaction source terms is negated in the species equations as species conservation by assuming the species diffusivities as the same. The scalars in the combustion system such as species fractions, density, and temperature are uniquely related to the mixture fraction(s) and the value of each mass fraction, density and temperature are determined from calculated values of mixture fraction, variance in mixture fraction and the enthalpy. The chemical species that were considered in the equilibrium calculations (CH₄, C₂H₂, CH₃, C₂N₂, C₂H₆, C₂H₄, C₄H₂, C₃H₃, HNC, C(s), CO, CO₂, H₂O, OH, N₂, O₂, H, O, HO₂ and H₂). This chemistry mechanism consists of 31 mixture fraction points with 20 species 41 mean enthalpy points with an assumed shape

probability distribution function (PDF) implicated to describe the turbulence-chemistry interactions where the average value of the scalars is related to mixture fraction data. In this study, the shape of the PDF was described by the beta function.

Turbulence Modeling

The turbulence was modeled using the realizable $k - \varepsilon$ model where the turbulence interaction was modeled as transported temperature variance. For the turbulence radiation interaction modeling we used a user defined function (UDF) to enhance the turbulence factor calculated from the analyzed data and including turbulence interaction mode with temperature PDF with 10 PDF points and using transported temperature variance.

CHAPTER IV

RESULTS AND DISCUSSION

In figure 6, the CO mole fraction contours of the five flames are shown up to a height of 125mm from the burner nozzle tip. The experimental flames are shown in Figure 7 for comparison. The numerically predicted flame spread is seen to be identical to the experimental flames. In Figure 10, the contours of CO mole fractions are shown since they are often chosen to characterize the flame lengths. The maximum CO mole fraction across all flames was numerically predicted to be 0.23. Therefore, the locus of points corresponding to the 1% of the peak value of CO was chosen to identify the flame shape and subsequently the flame length. Mei et al [16, 17] in their simulations of turbulent oxy-methane flames, looked at various ways of defining a flame length and deemed the 1% of maximum CO mole fraction as the most accurate representation of the flame length in oxy-flames.

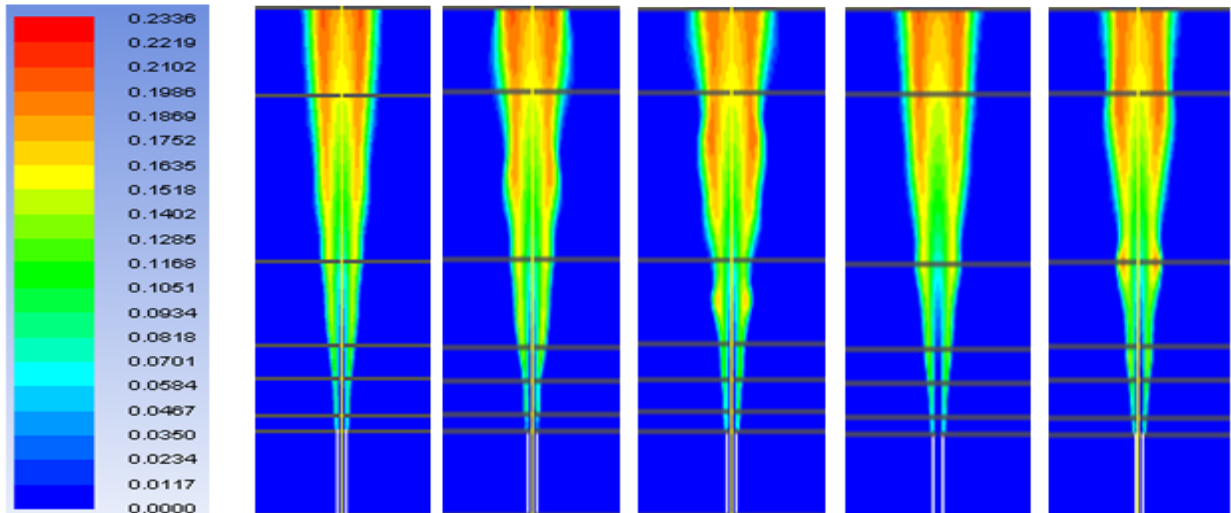


Figure 6: Contours of CO specie shown upto 125mm for the lengths of flames A to E indicated from left to right (the lines indicating flame length $z=0$ mm, $z=5$ mm, $z=15$ mm, $z=25$ mm, $z=50$ mm and $z=100$ mm and the top of the length is $z=125$ mm)

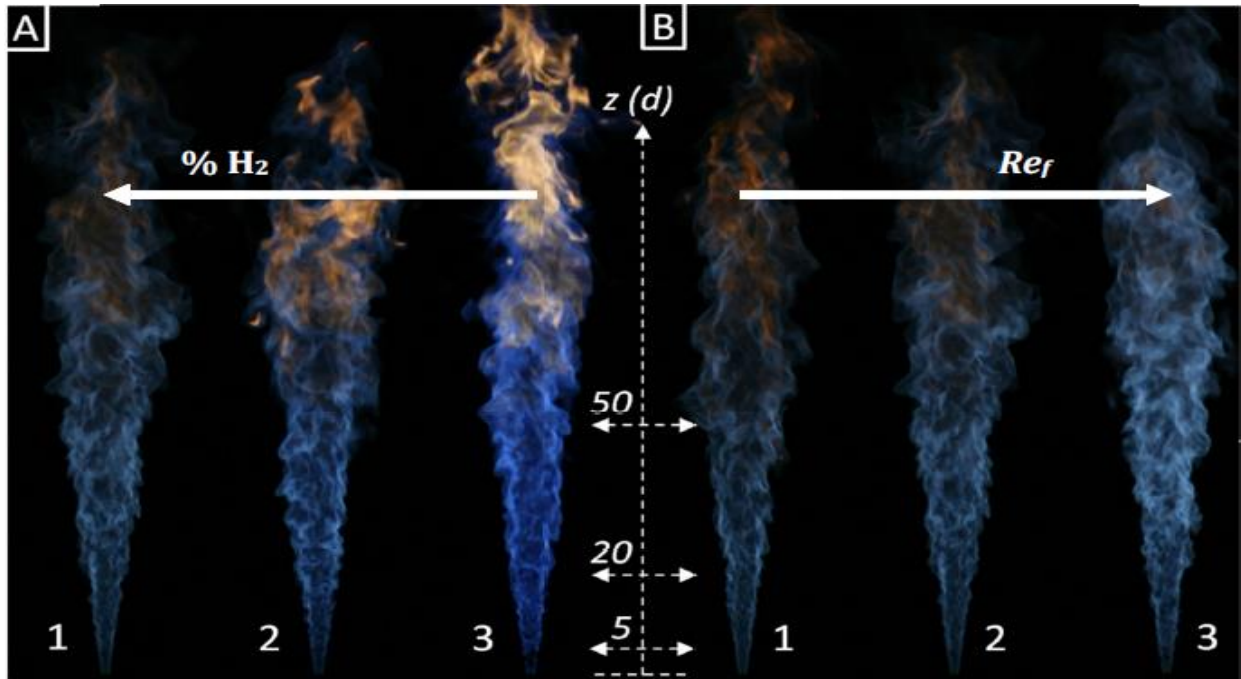


Figure 7: Experimental figures of five flames (from figure A-1 & B-2 are the same flames) sequentially from A to E according to directed in figure 6 (Sevault Dissertation, 2012)

From the table 2 we observed that for flames A, B and C the fuel composition was changed keeping the fuel velocity same. We find that the flame temperature varies with the fuel composition change. For flames D, A and E respectively the Reynolds number was changed by

Flames	Temperature (K) Without Radiation Condition	Fuel Composition CH ₄ /H ₂ (%mol)	Temperature (K) With Radiation condition	Reynolds number (Re _f)	∇Trad (K)
A	1994	45/55	1901	15000	-93
B	1968	55/45	1913	15000	-55
C	1956	63/37	1958	15000	2
D	1983	45/55	1898	12000	-85
E	2510	45/55	1925	18000	-585

Table 2: Computed flame peak temperature

changing the jet velocity. To keep pace with the fuel jet velocity and to provide proper mixing the co-flow velocity was also varied accordingly which was shown in table 1.

The flame lengths were determined by separating out the flame region by computed CO species taking the peak value as the maximum and 1% of the peak value as minimum [Mei et al, 2015].

The flame regions are shown in the figure 12 and the lengths are calculated by separating out the cells of CO contour region from the flow field. The lengths of the flames are shown in table 3.

The numerical prediction of the flame length contours defined in this manner is shown in Figure 8 and the numerical values of the flame length are reported in Table 3. For Flames A – C where the Reynolds number is fixed, with a decrease in H₂ mole fraction in the fuel stream, the flame length increases. This is likely because the presence of H₂ in the fuel stream increases the flame temperature and increases the reaction rates, therefore completing the reactions at lower axial distances. For flames D, A and E where the fuel composition stays the same but the Reynolds number increases, we notice a slight decrease in flame lengths. In reality, the flame lengths remain nearly the same in the turbulent regime and these are likely due to numerical differences.

From Figure 7, the experimentally observed flame lengths were observed to be at z/d ratios of 100 – 125 i.e., corresponding to heights of 500 to 625 mm. Therefore, the numerically predicted heights are in agreement with experimental observations. The peak temperatures predicted by the flames are shown in Table 2. A set of calculations were also carried out without invoking the radiation model and the peak predicted temperatures associated with those calculations are also shown. Emission losses due to radiative transfer results in flame cooling and results in a cooler flame temperature up to nearly 100 K in some flames. This can result in significant variations in prediction of pollutants such as NO_x and CO.

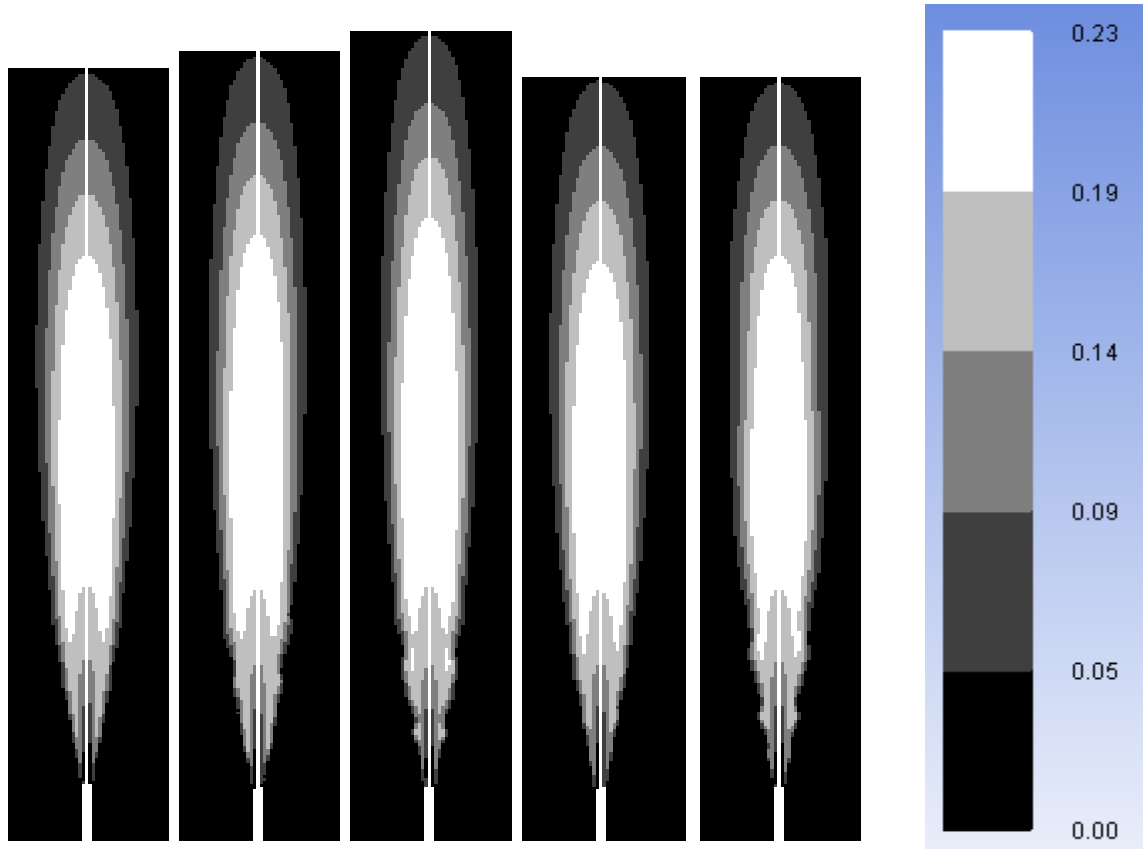
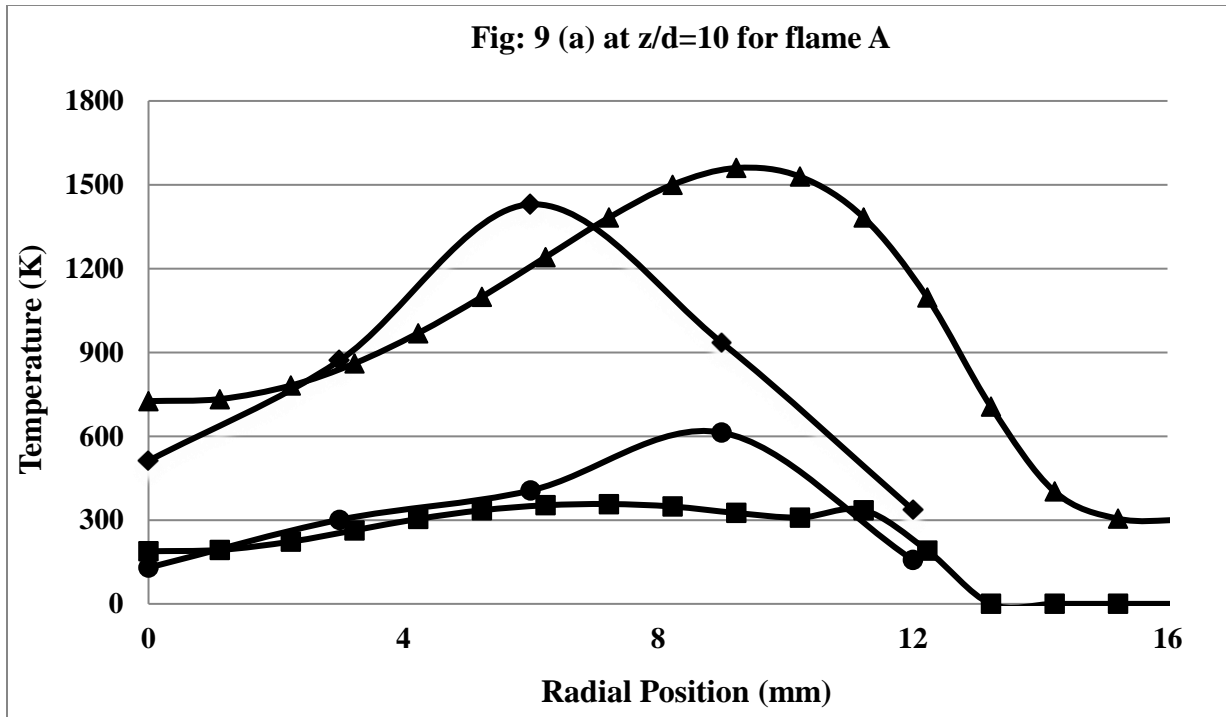


Figure 8: Flame region of the five simulated flames shown through the contours of mole fraction of CO (from left through right A to E)

Flame	A	B	C	D	E
Height (mm)	529	547	560	532	523

Table 3: Calculated flame lengths from simulations

In figures 9-13, the predicted radial variations in the mean temperature and Trms at different axial locations across all flames are compared against the experimental measurements. A reasonable agreement between the experimental measurements and the numerical predictions is observed across all flames providing credibility to our modeling procedure. Later we have shown in figures 14-18 (temperature vs radial position) and 19-23 (CO₂ vs radial position) showing the simulated values within the range of a standard deviation of the calculated experimental mean.



Tavg, exp
 Trms, exp
 Tavg, sim
 Trms, sim

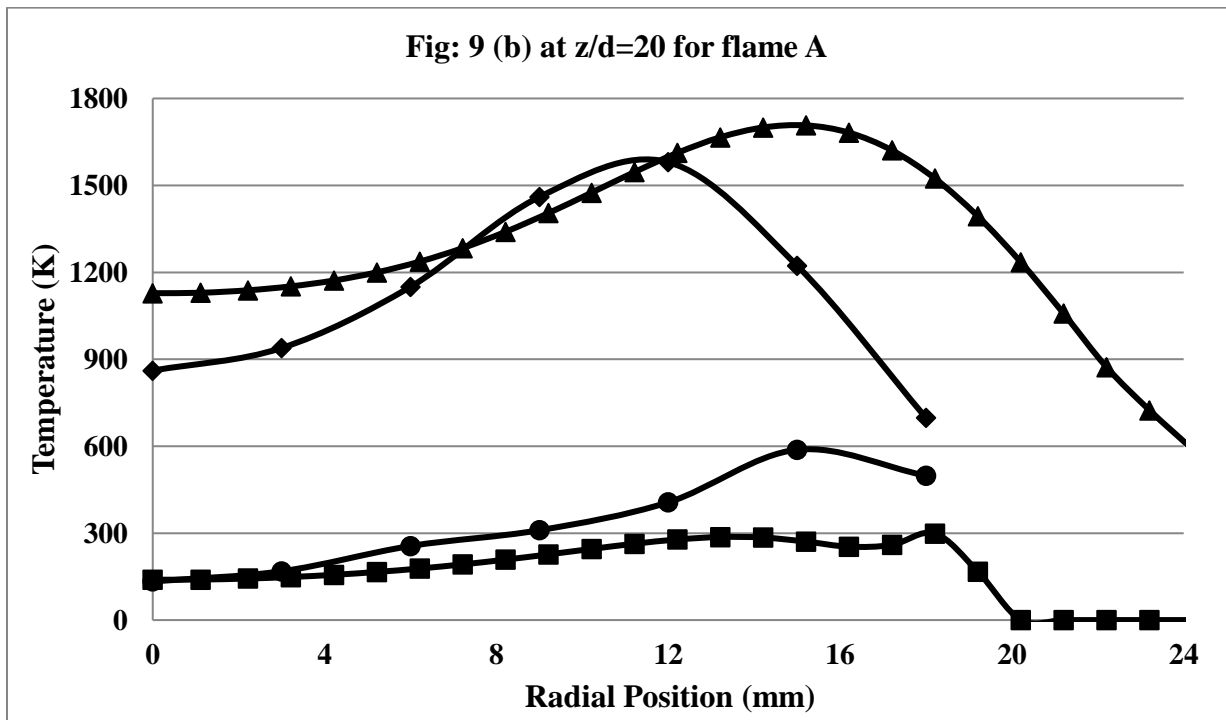
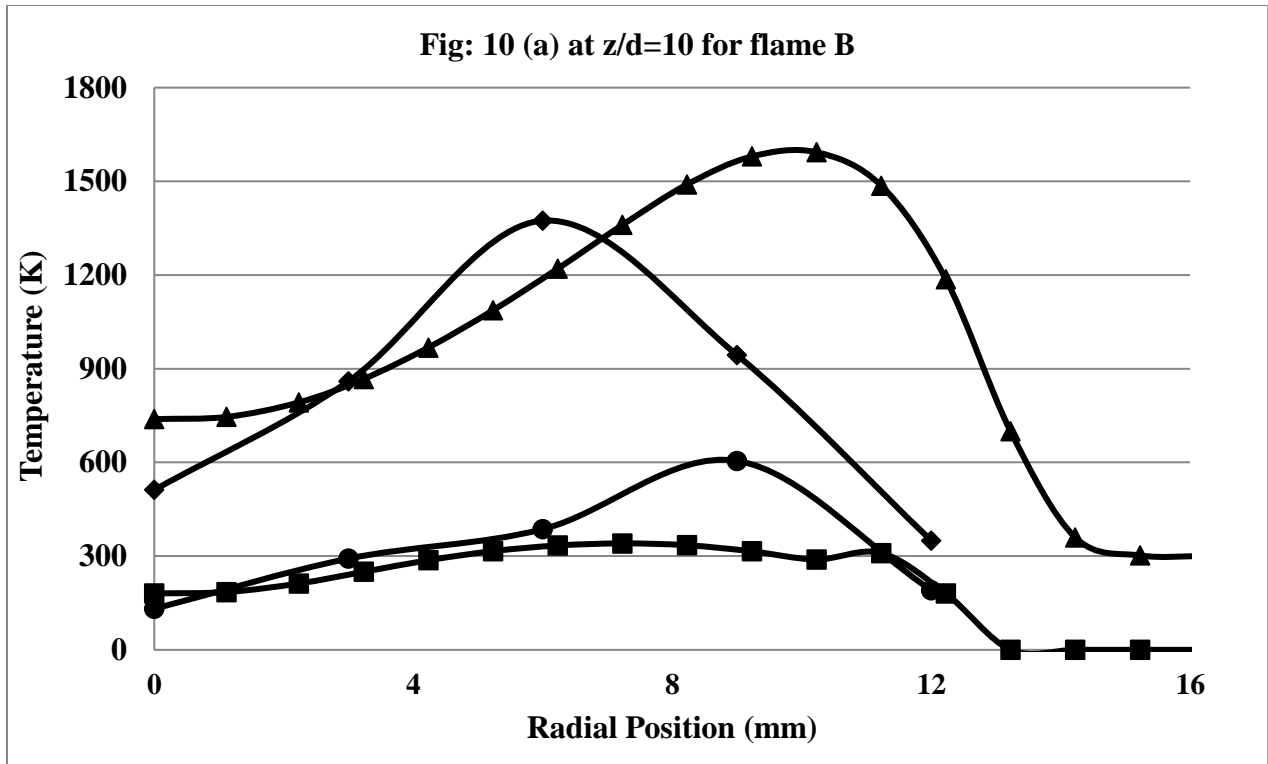


Figure 9: Tmean, Trms Vs radial position at z/d=10 and z/d=20 of flame A for experimental and simulated conditions without TRI



◆ Tavgs, exp ● Trms, exp ▲ Tavgs, sim ■ Trms, sim

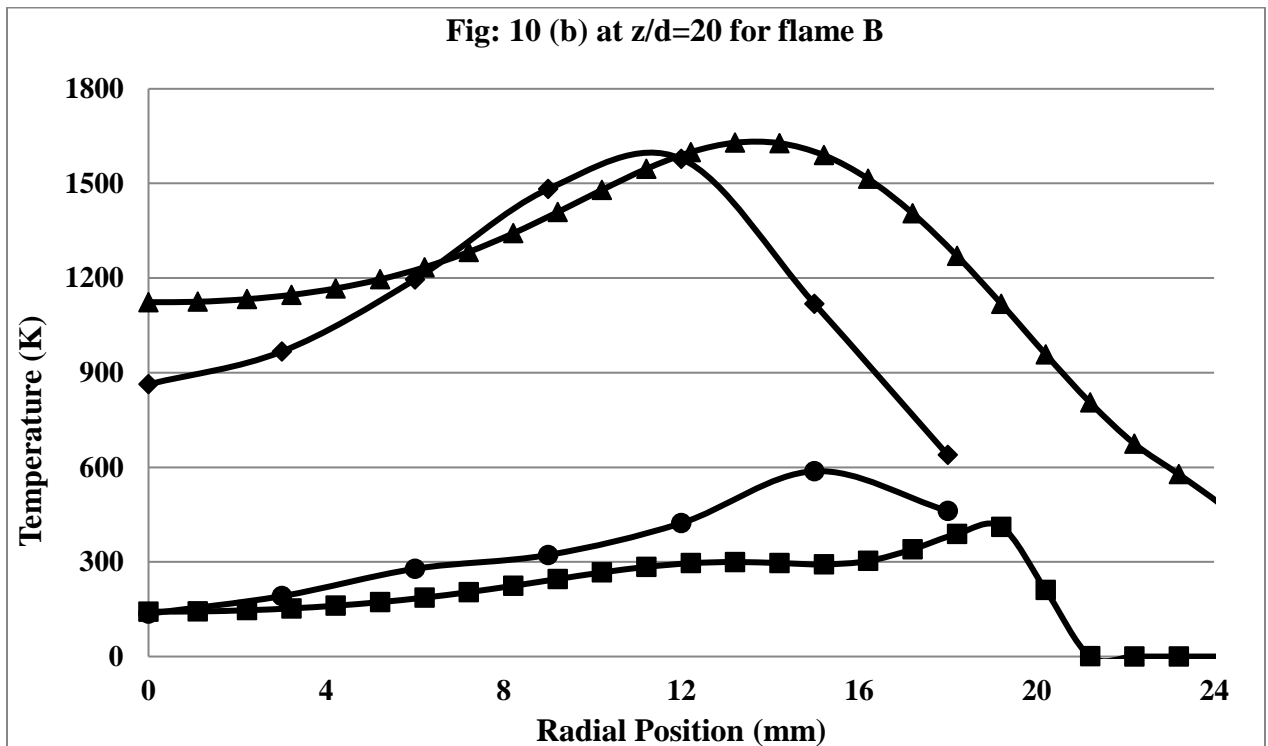
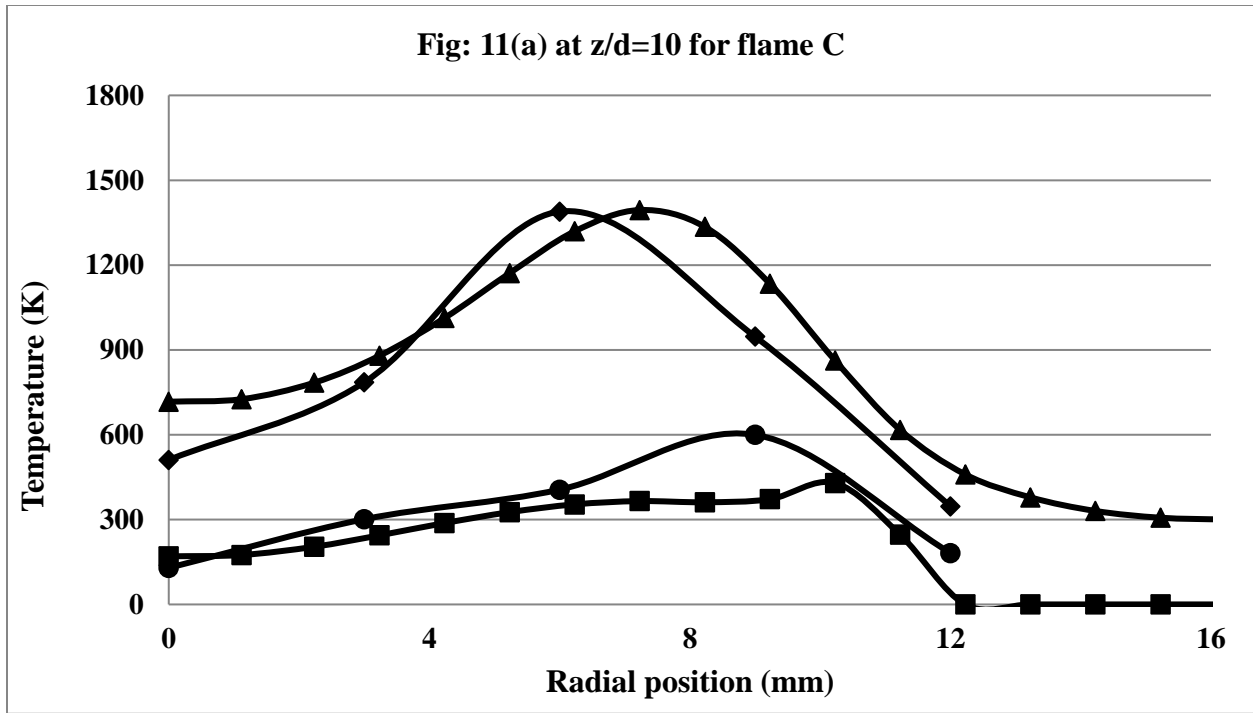


Figure 10: Tmean, Trms Vs radial position at $z/d=10$ and $z/d=20$ of flame B for experimental and simulated conditions without TRI



Tavg, exp
 Trms, exp
 Tavg, sim
 Trms, sim

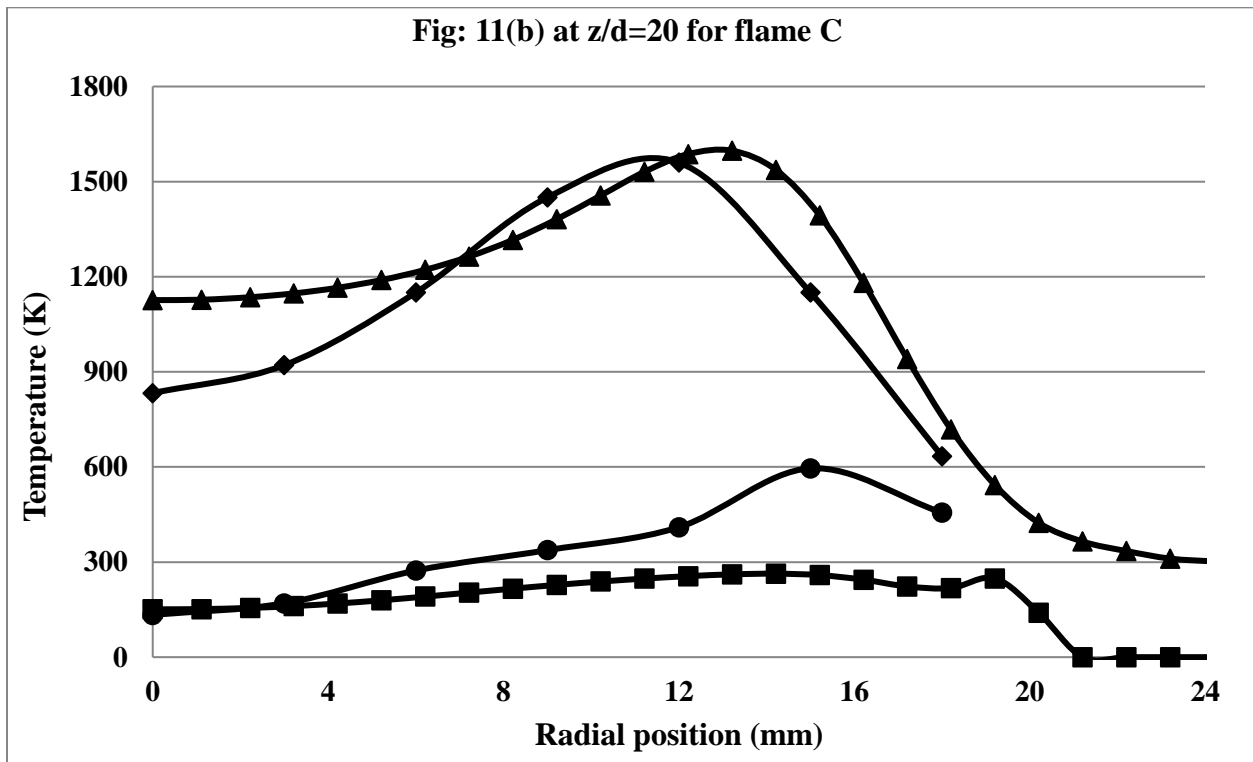
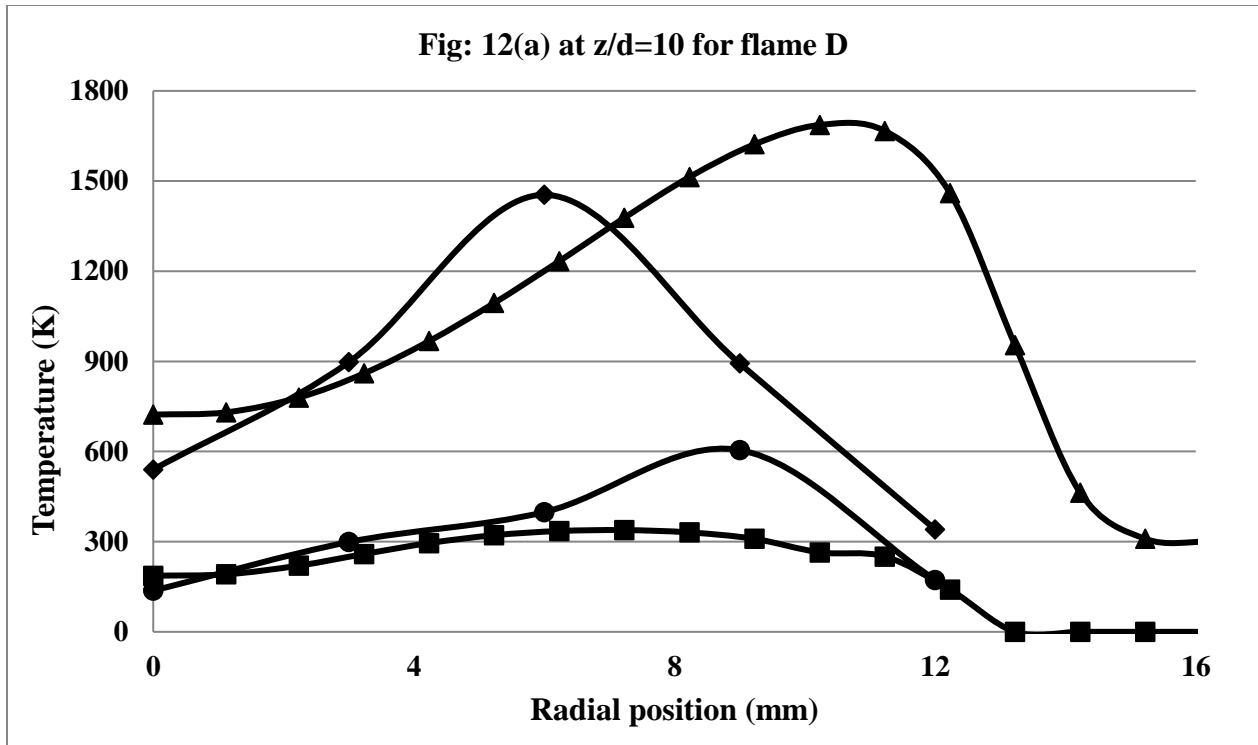


Figure 11: Tmean, Trms Vs radial position at $z/d=10$ and $z/d=20$ of flame C for experimental and simulated conditions without TRI



Tavg, exp
 Trms, exp
 Tavg, sim
 Trms, sim

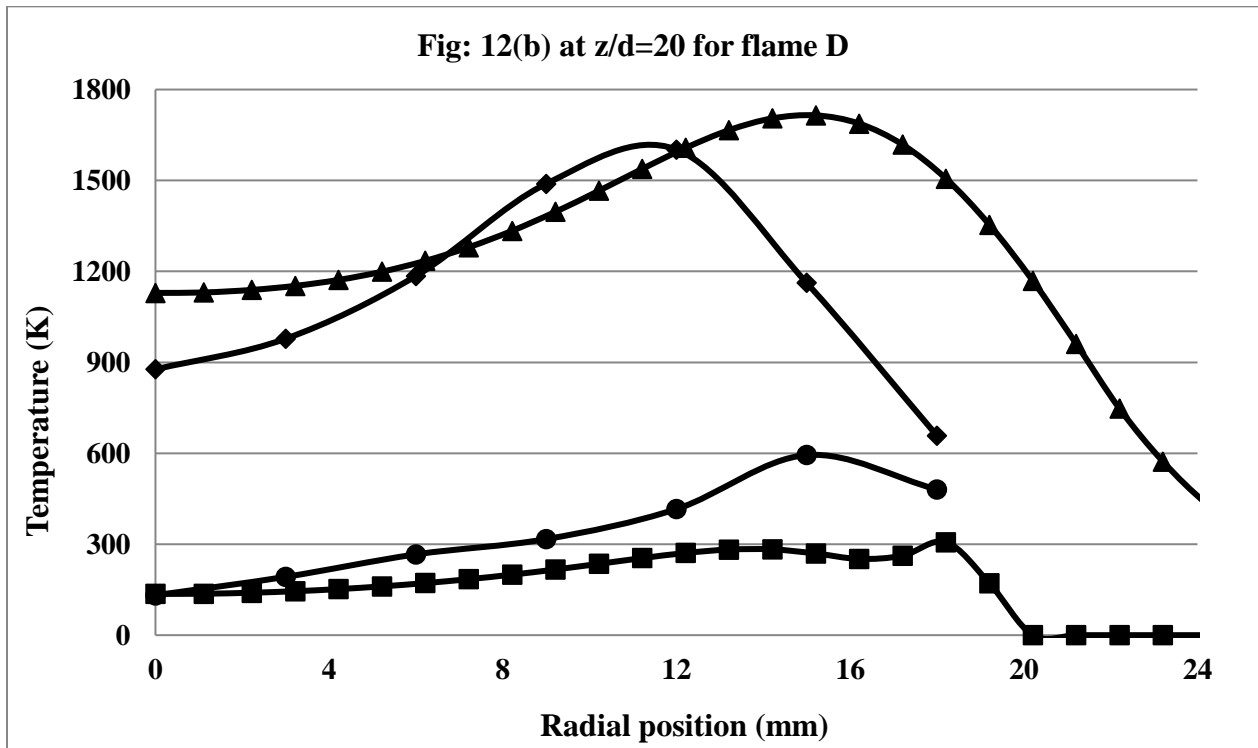
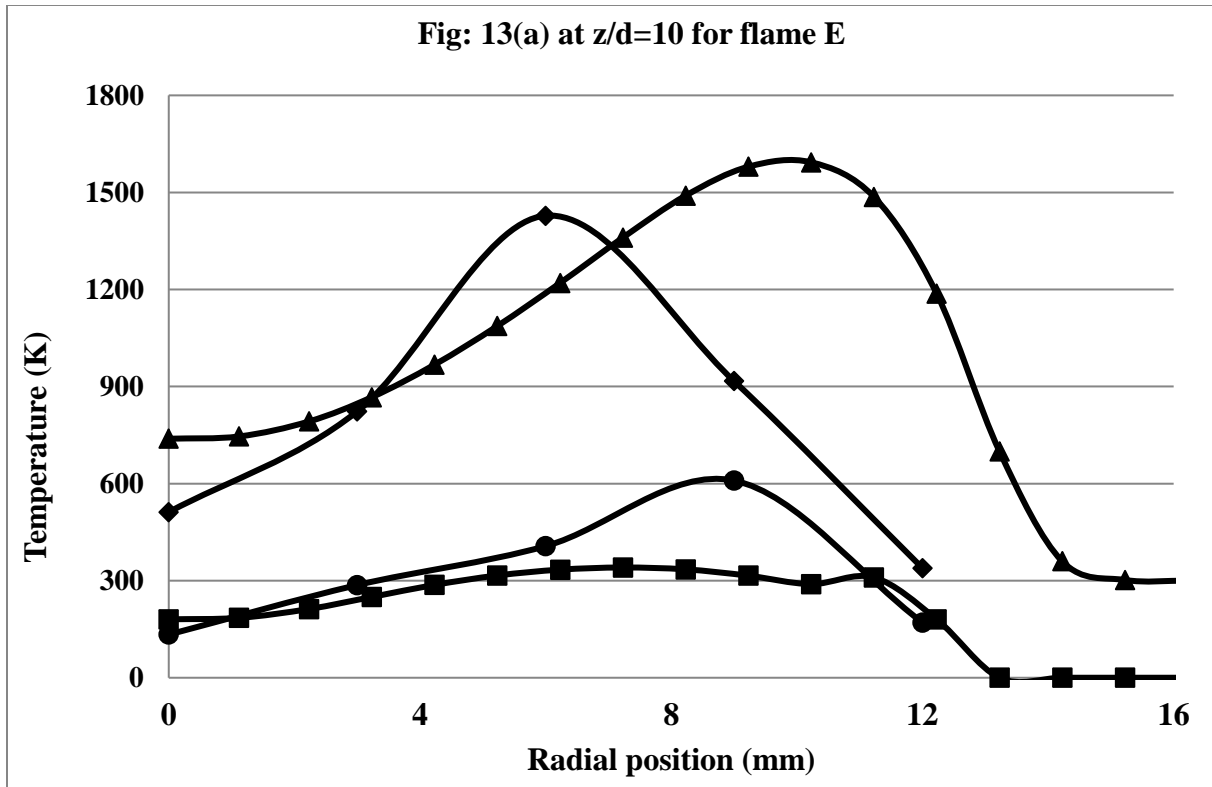


Figure 12: Tmean, Trms Vs radial position at $z/d=10$ and $z/d=20$ of flame D for experimental and simulated conditions without TRI



◆ $T_{avg, exp}$ ● $T_{rms, exp}$ ▲ $T_{avg, sim}$ ■ $T_{rms, sim}$

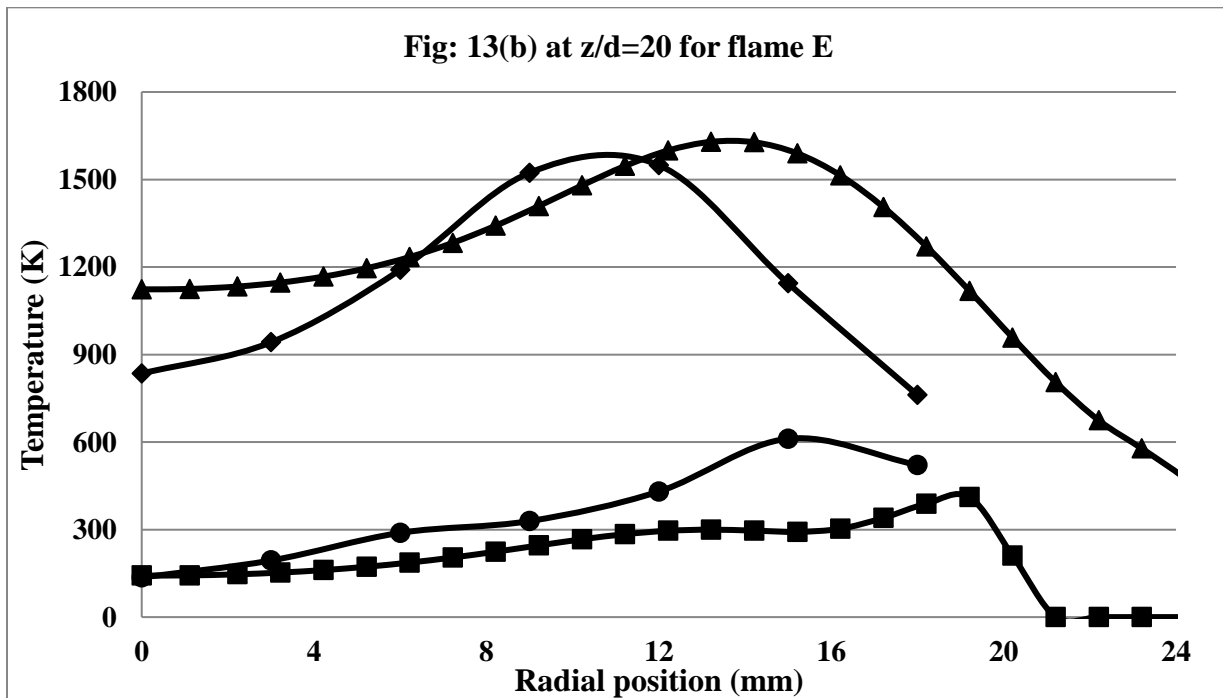


Figure 13: T_{mean} , T_{rms} Vs radial position at $z/d=10$ and $z/d=20$ of flame E for experimental and simulated conditions without TRI

Figures 14-18 and figures 19-23 shows the experimental vs simulated flame temperatures and CO₂ specie values respectively along the radial axis at 50mm ($z/d=10$) position and at 100mm ($z/d=20$) position. The mean values of the experimental temperatures are shown along with the upper and lower standard deviation values of the mean values. From these figures we can conclude that the simulated cases in comparison with the actual experimental results do not differ a lot and falls within the range of one standard deviation as calculated as a whole. Though there are variations in the temperature and CO₂ specie field according to the figures shown under figures 14-18 and figures 19-23 for different positions and different flame conditions are seen the variations are seen within the range of one standard deviation. An improved agreement could be obtained by resolving the turbulence and gas-phase chemistry better.

To include the turbulence radiation interaction into the RANS (Reynolds Averaged Navier Stokes) simulation is a very difficult task. From equation (5) we see that the slope of the temperature self-correlation equation should be 6. But in FLUENT code in RANS modeling because of the turbulence fluctuations are not considered the slope is 0 indicating that the turbulence temperature and mean temperature in each position of the flow field are same. So a primary goal of this thesis is to use experimental data to resolve and model the turbulence radiation interaction through using user defined functions (UDF). Detailed statistical data analysis was done from the experimental results to find out the impact of various interactions towards the turbulence radiation interaction. Analyzing the temperature self-correlation versus the temperature fluctuation intensity from experimental measurements helps us to incorporate the effects TRI as UDF into the simulations.

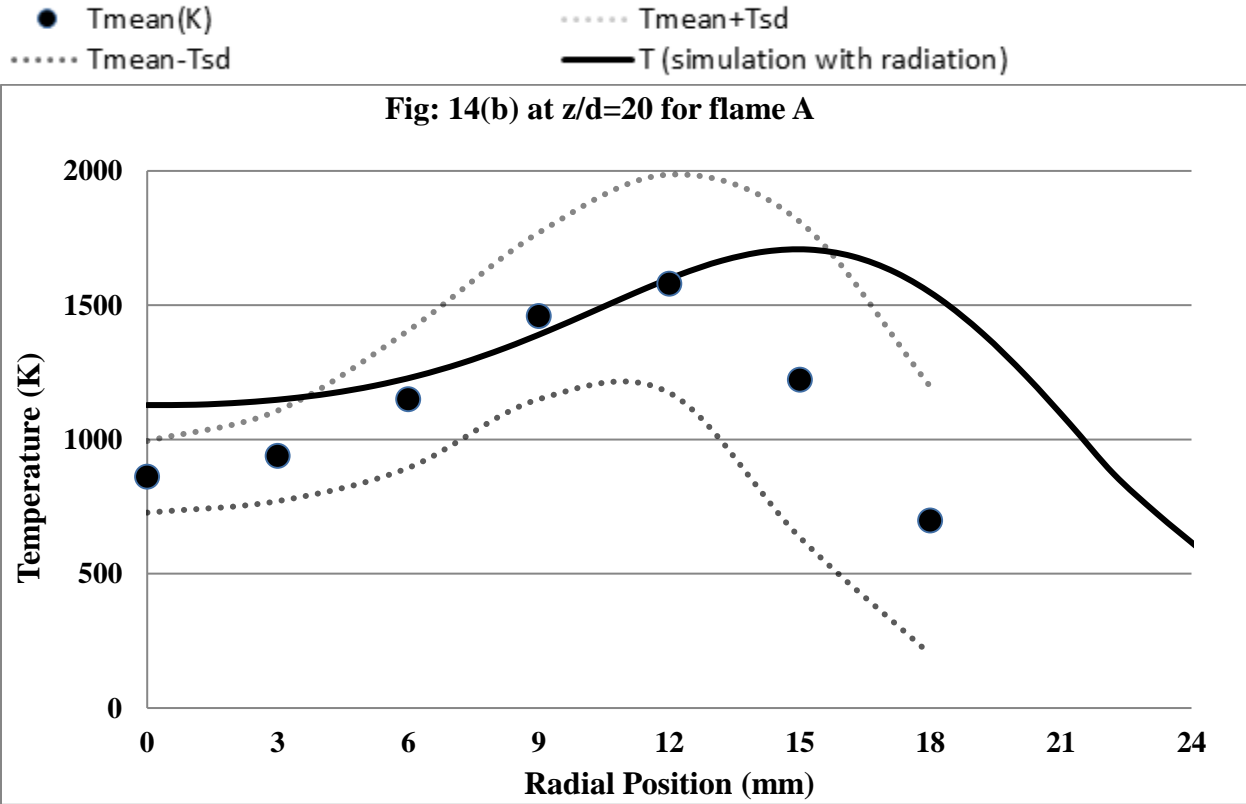
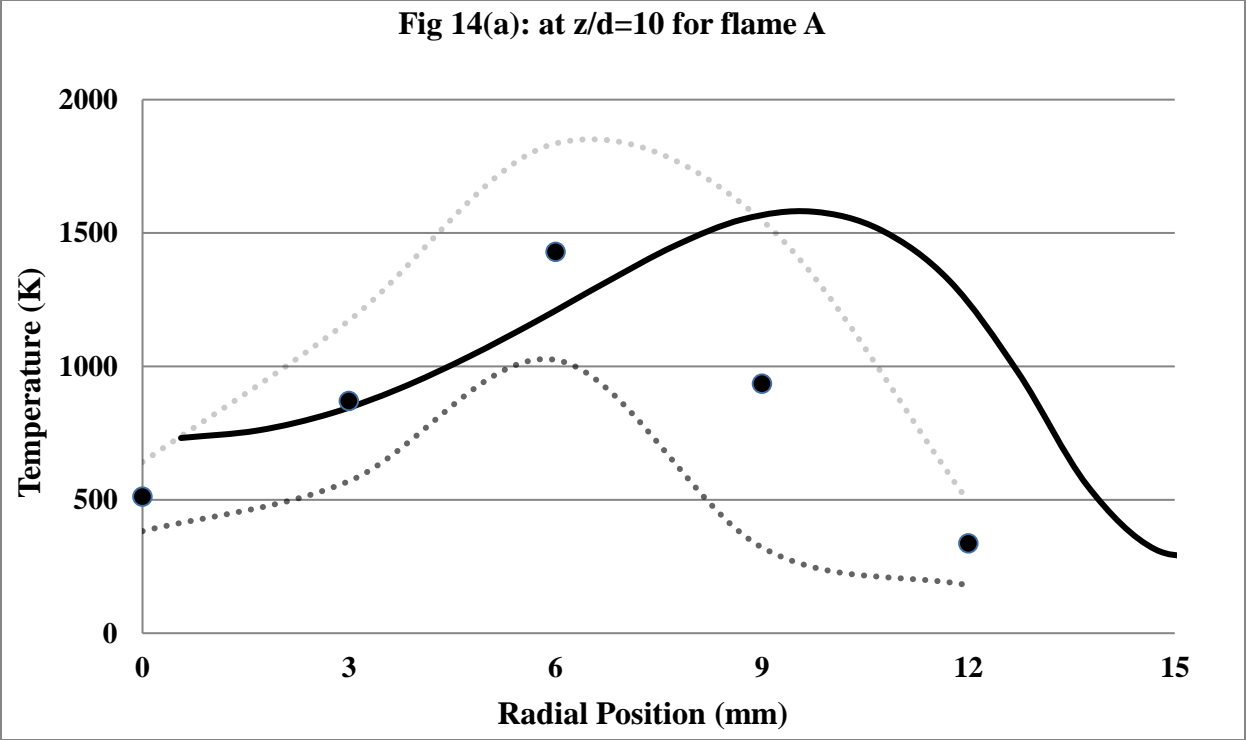


Figure 14: Radial profile of temperature at heights 50mm (left) and 100mm (right) from fuel nozzle outlet for flame A

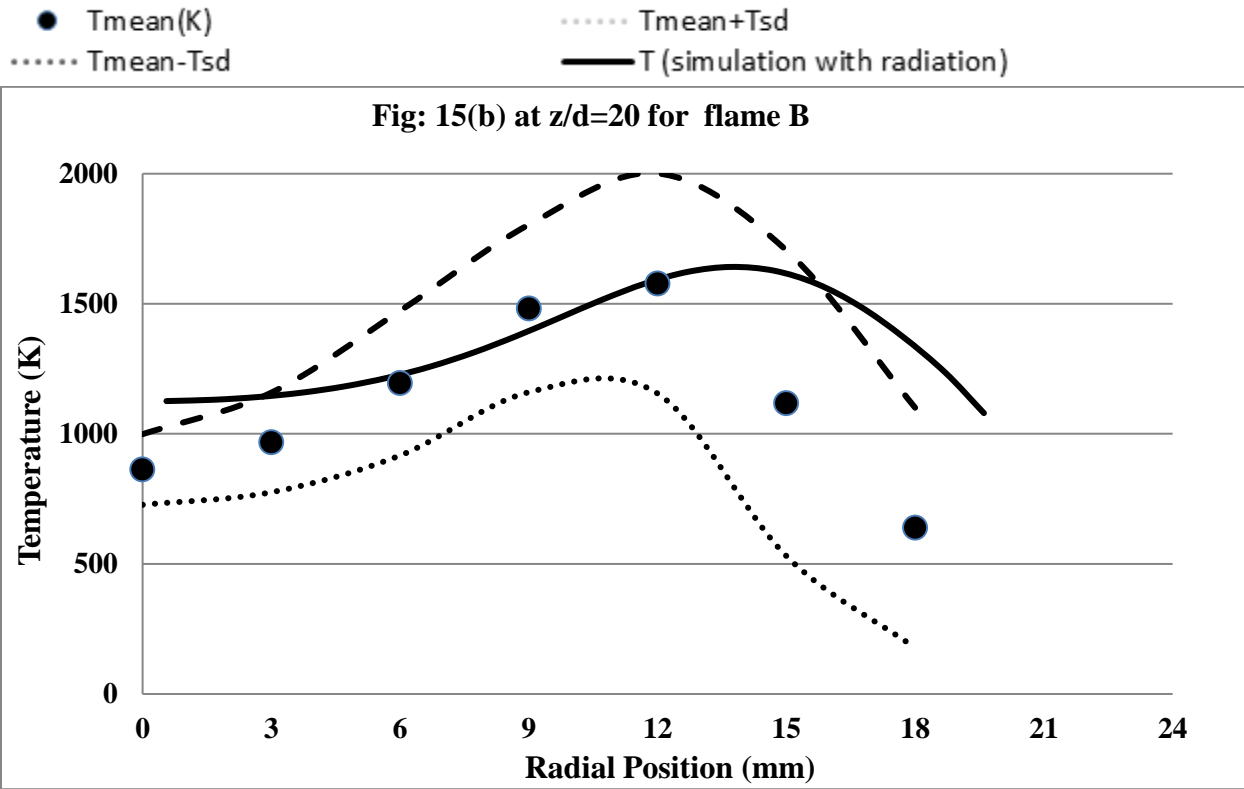
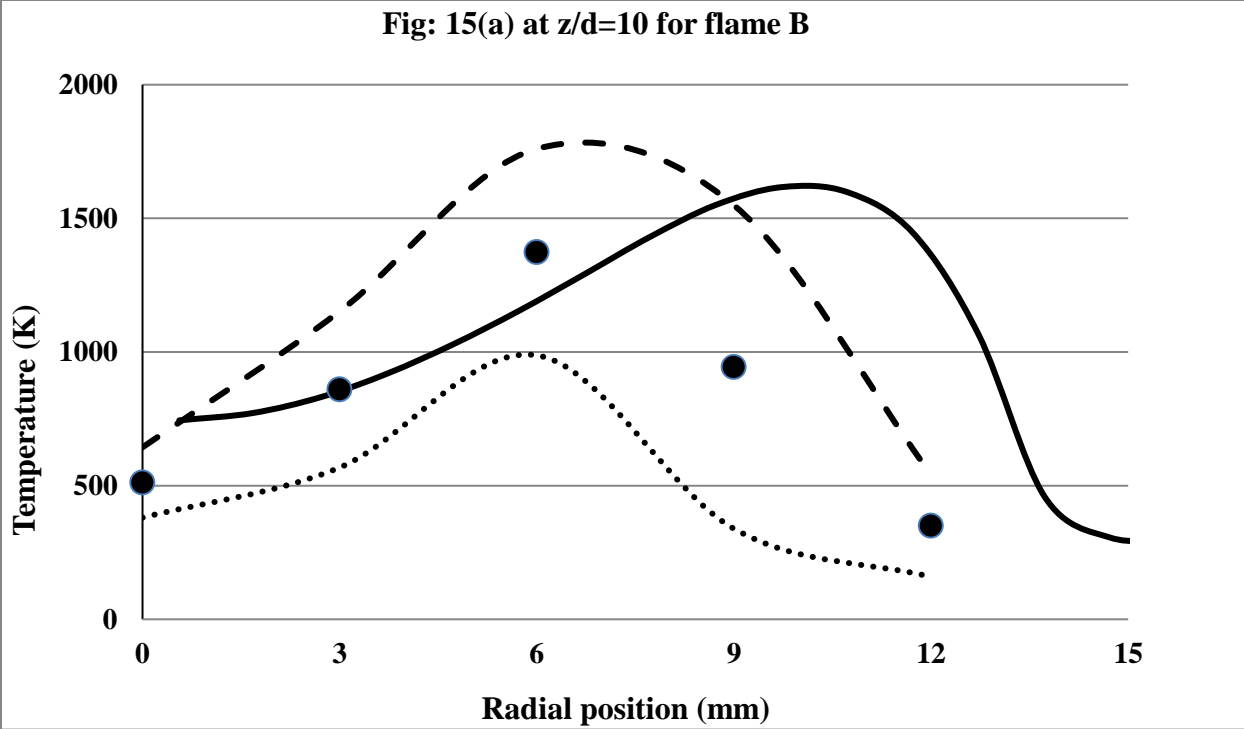


Figure 15: Radial profile of temperature at heights 50mm (left) and 100mm (right) from fuel nozzle outlet for flame B

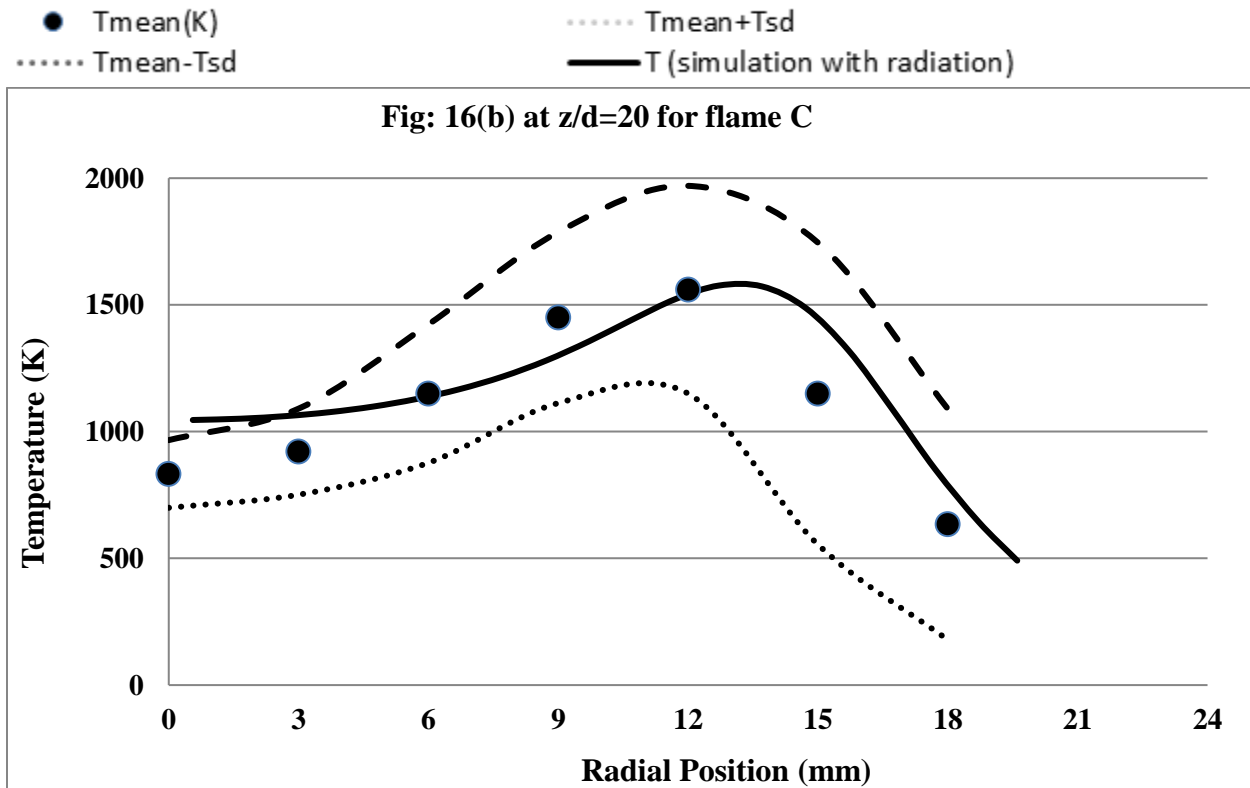
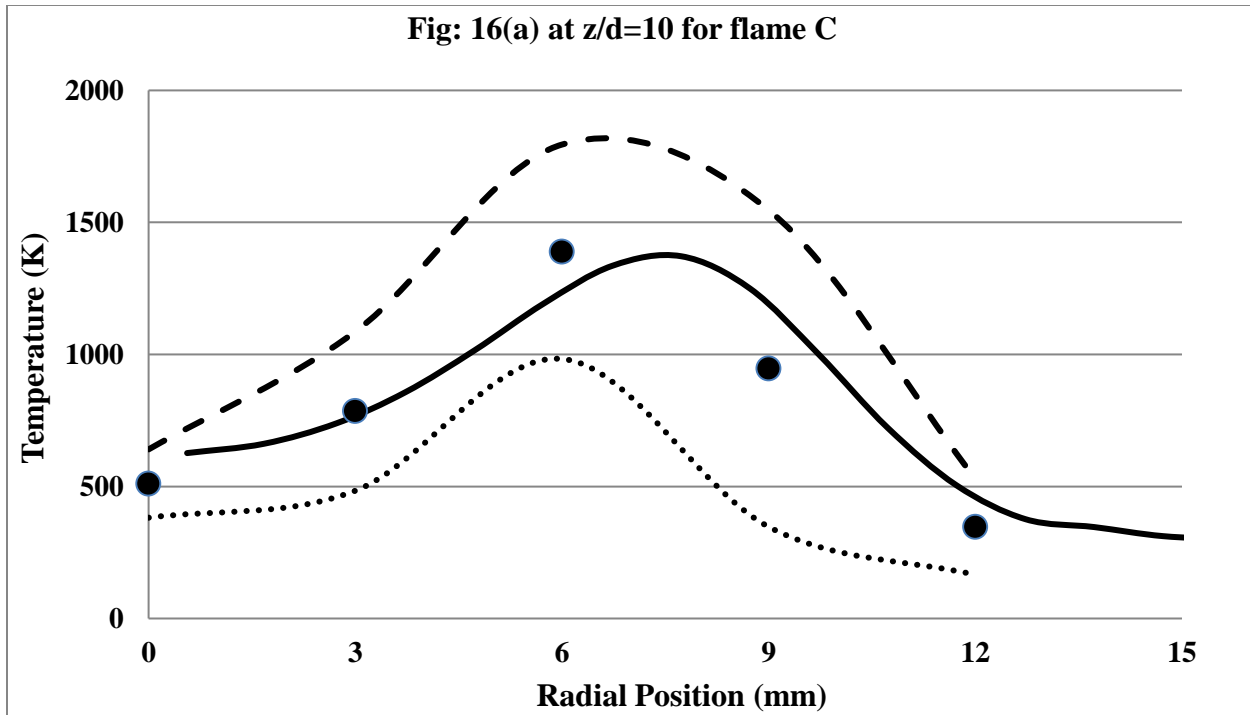


Figure 16: Radial profile of temperature at heights 50mm (left) and 100mm (right) from fuel nozzle outlet for flame C

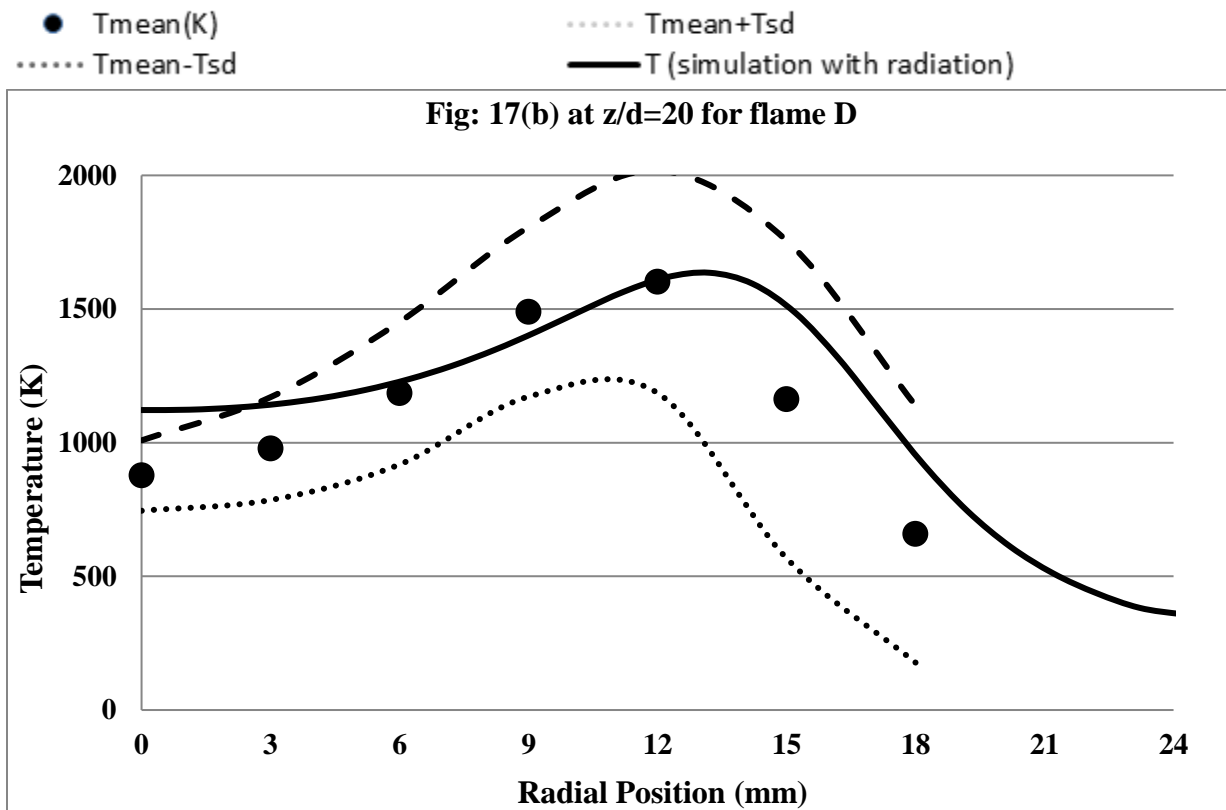
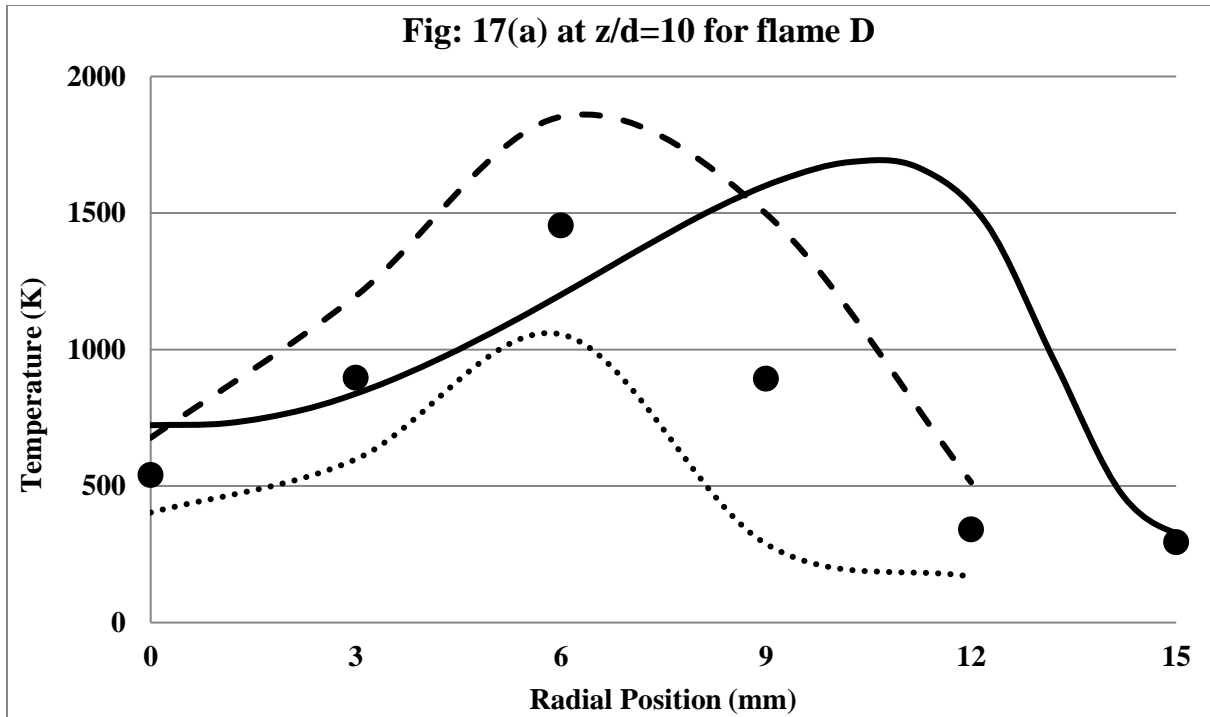


Figure 17: Radial profile of temperature at heights 50mm (left) and 100mm (right) from fuel nozzle outlet for flame D

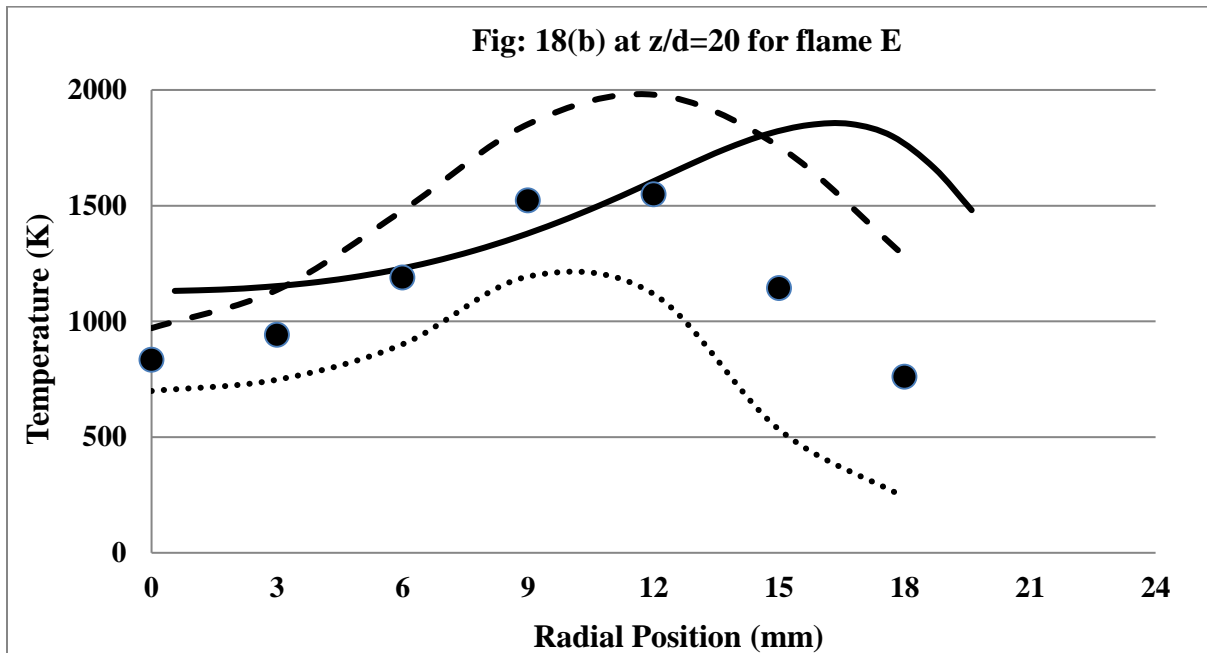
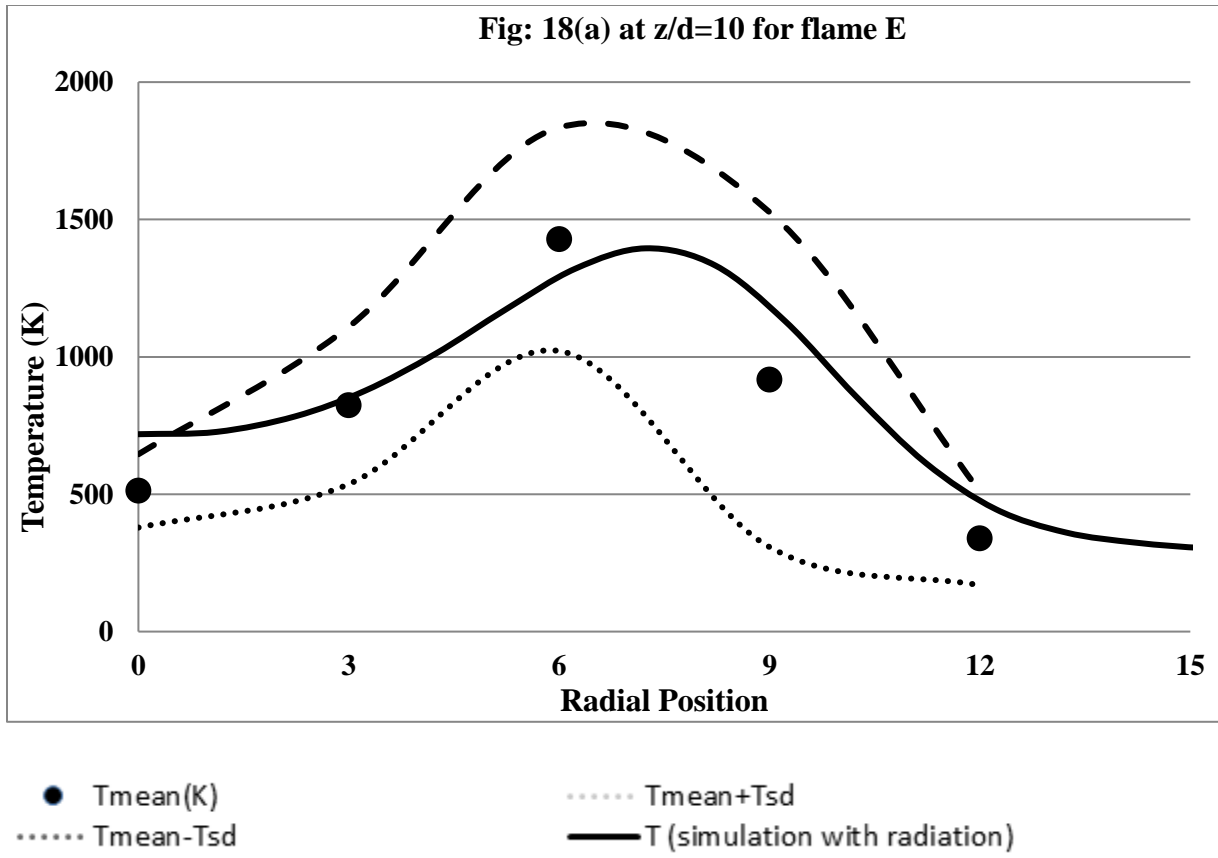
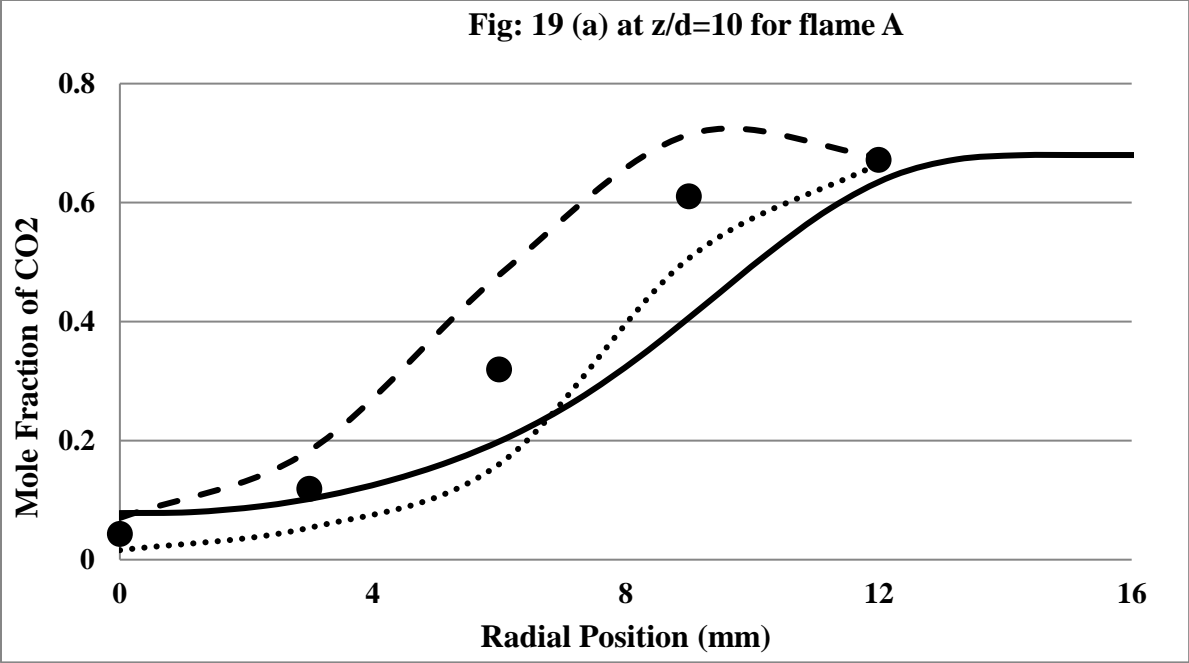


Figure 18: Radial profile of temperature at heights 50mm (left) and 100mm (right) from fuel nozzle outlet for flame E



CO2 mean
 CO2 (mean+sd)
 CO2 (mean-sd)
 CO2 (simulation with radiation)

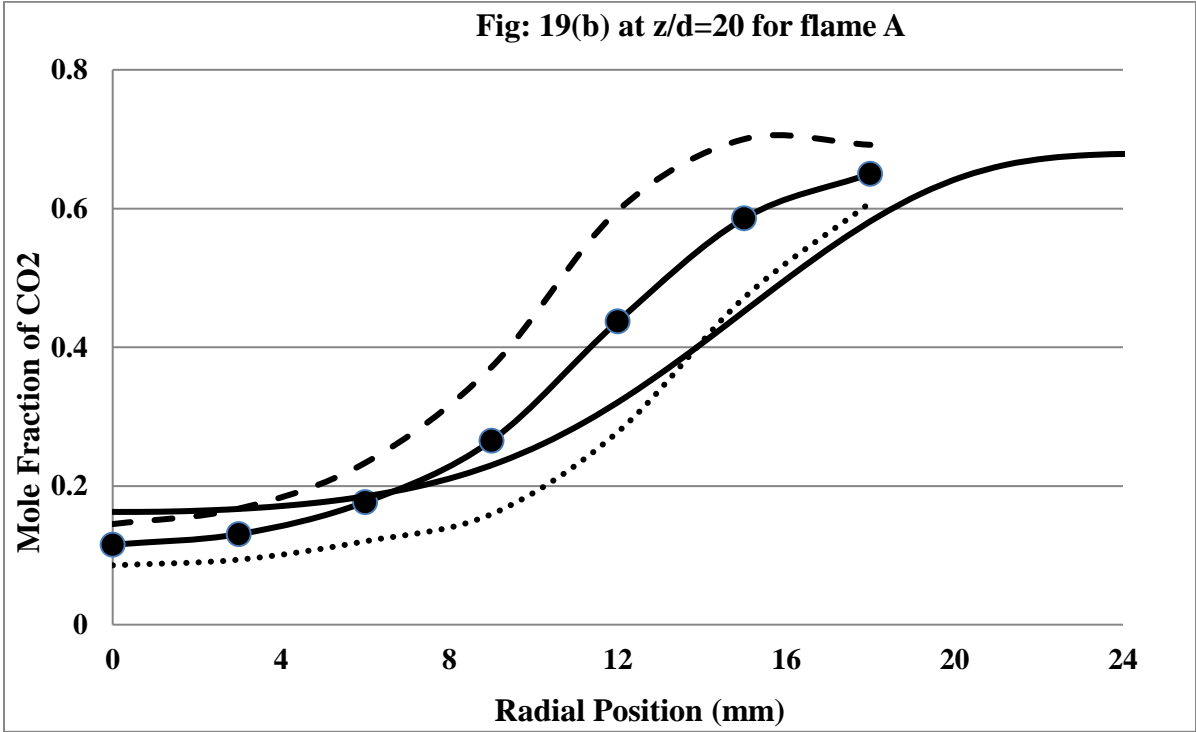
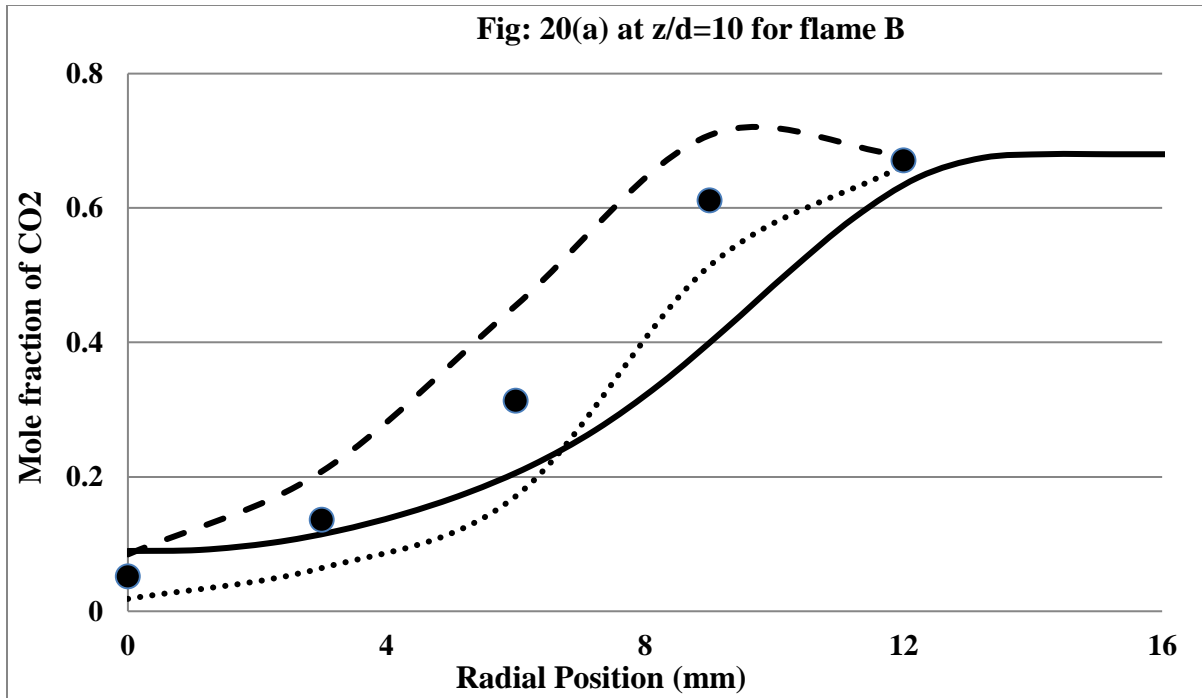


Figure 19: Radial profile distribution of CO₂ mole fraction at 50mm and 100mm height from the fuel nozzle for flame A



CO2 mean
 CO2 (mean+sd)
 CO2 (mean-sd)
 CO2 (simulation with radiation)

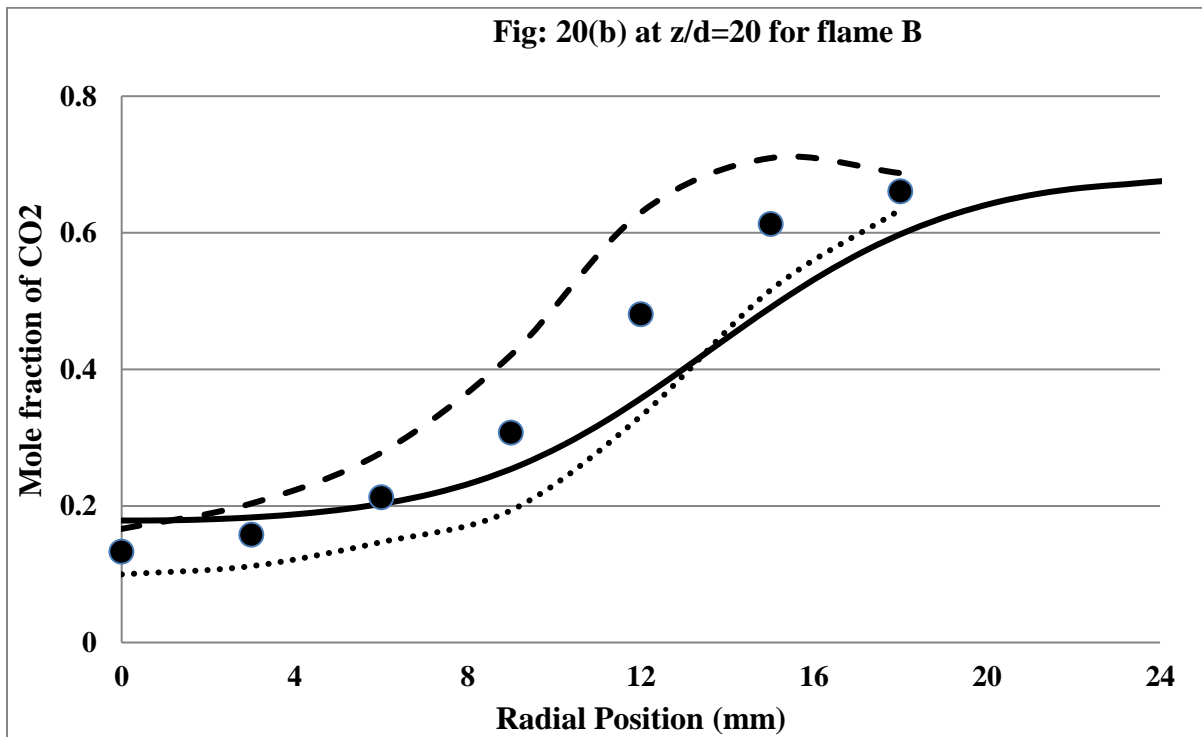
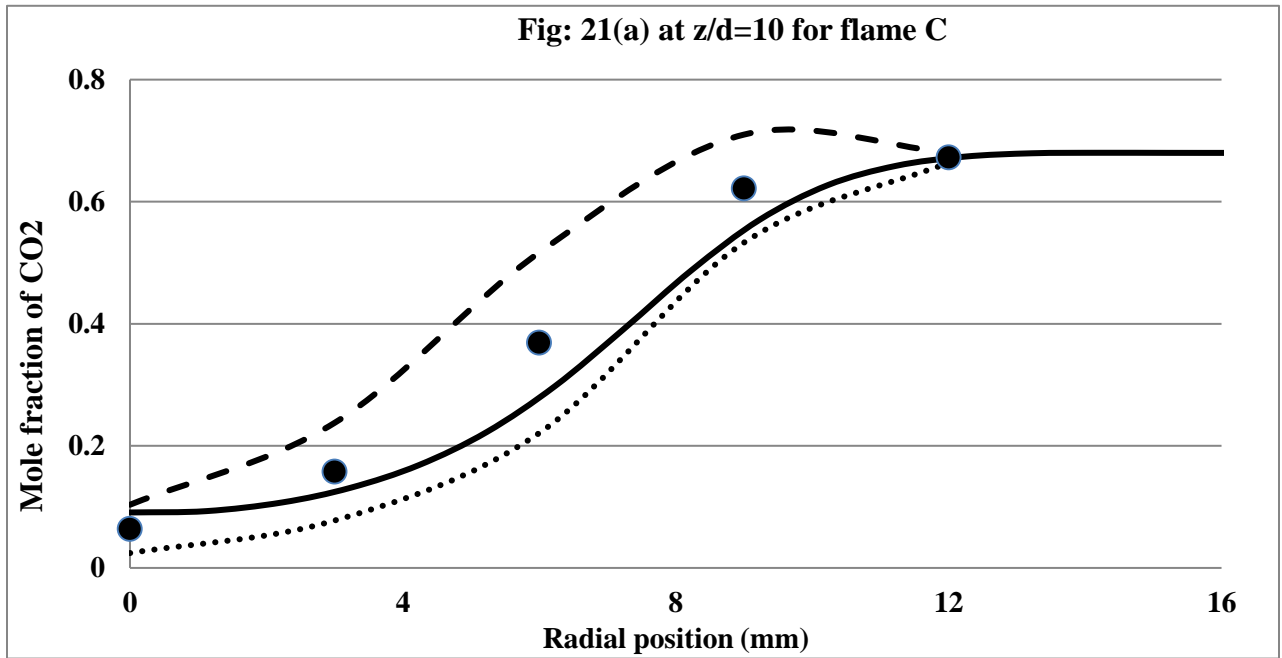


Figure 20: Radial profile distribution of CO₂ mole fraction at 50mm and 100mm height from the fuel nozzle for flame B



CO2 mean
 CO2 (mean+sd)
 CO2 (mean-sd)
 CO2 (simulation with radiation)

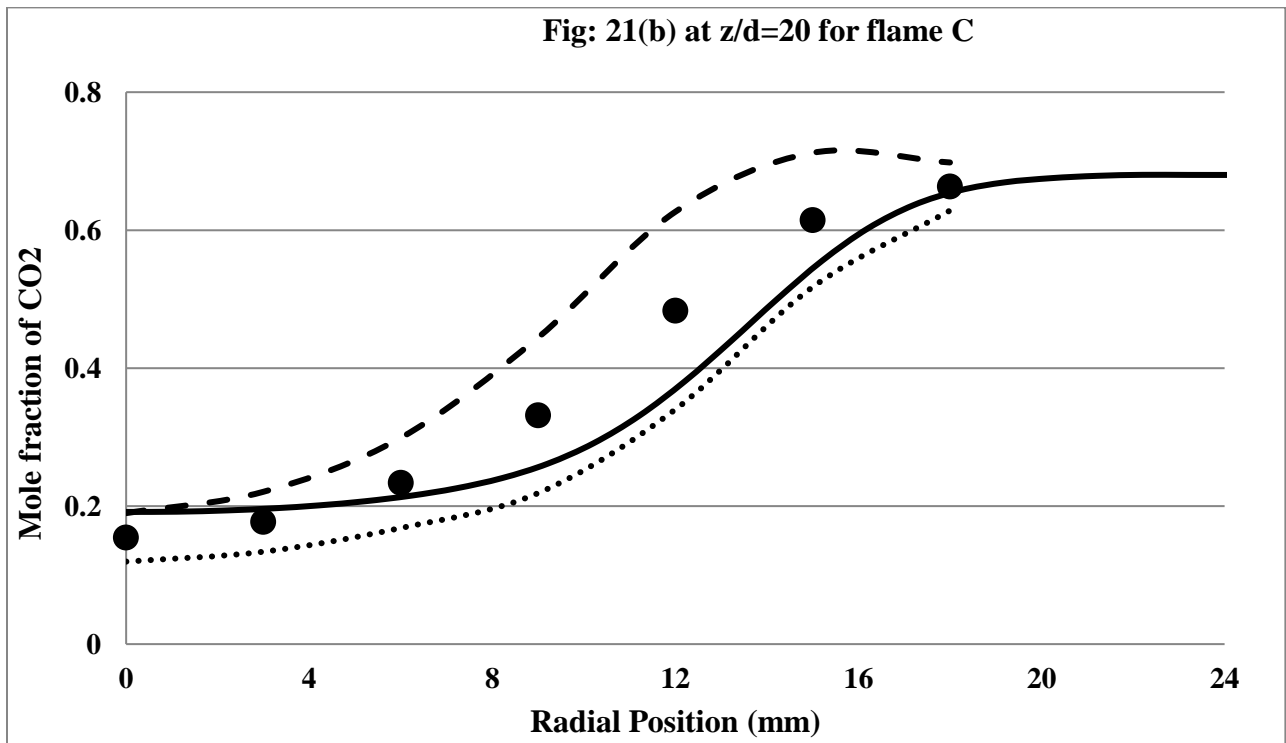


Figure 21: Radial profile distribution of CO₂ mole fraction at 50mm and 100mm height from the fuel nozzle for flame C

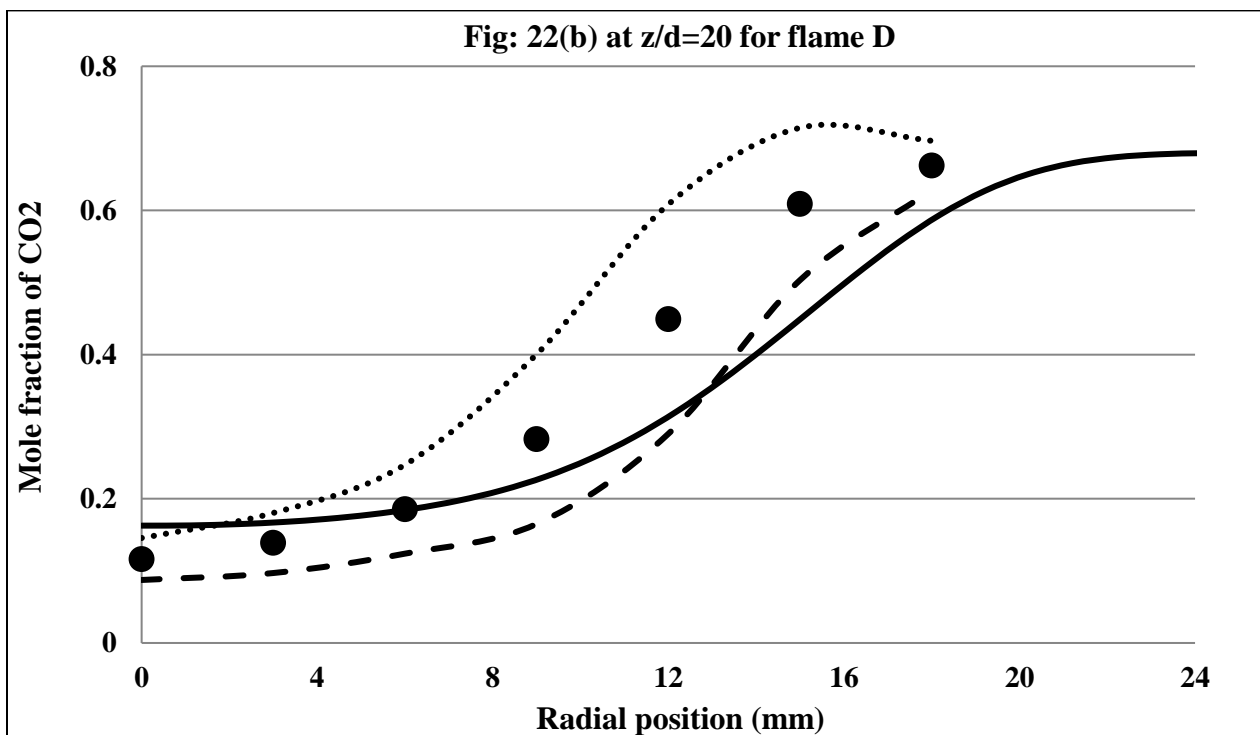
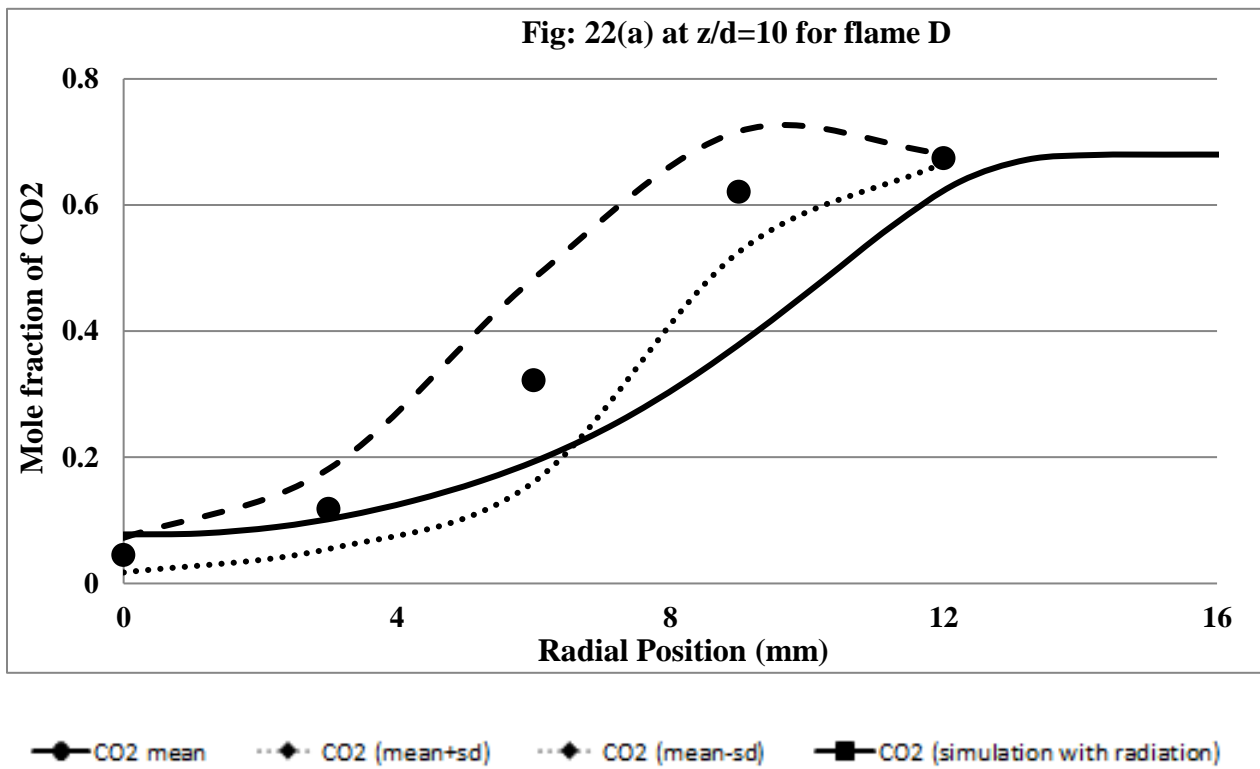


Figure 22: Radial profile distribution of CO₂ mole fraction at 50mm and 100mm height from the fuel nozzle for flame D

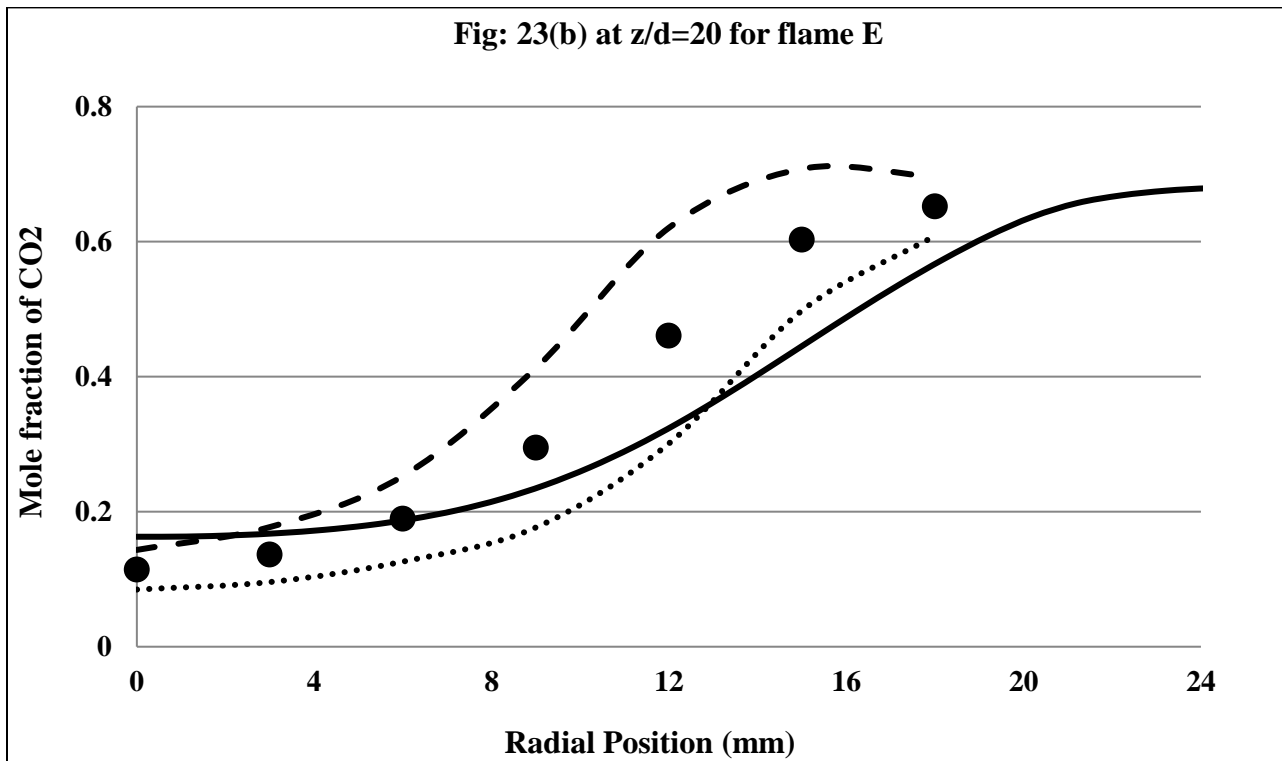
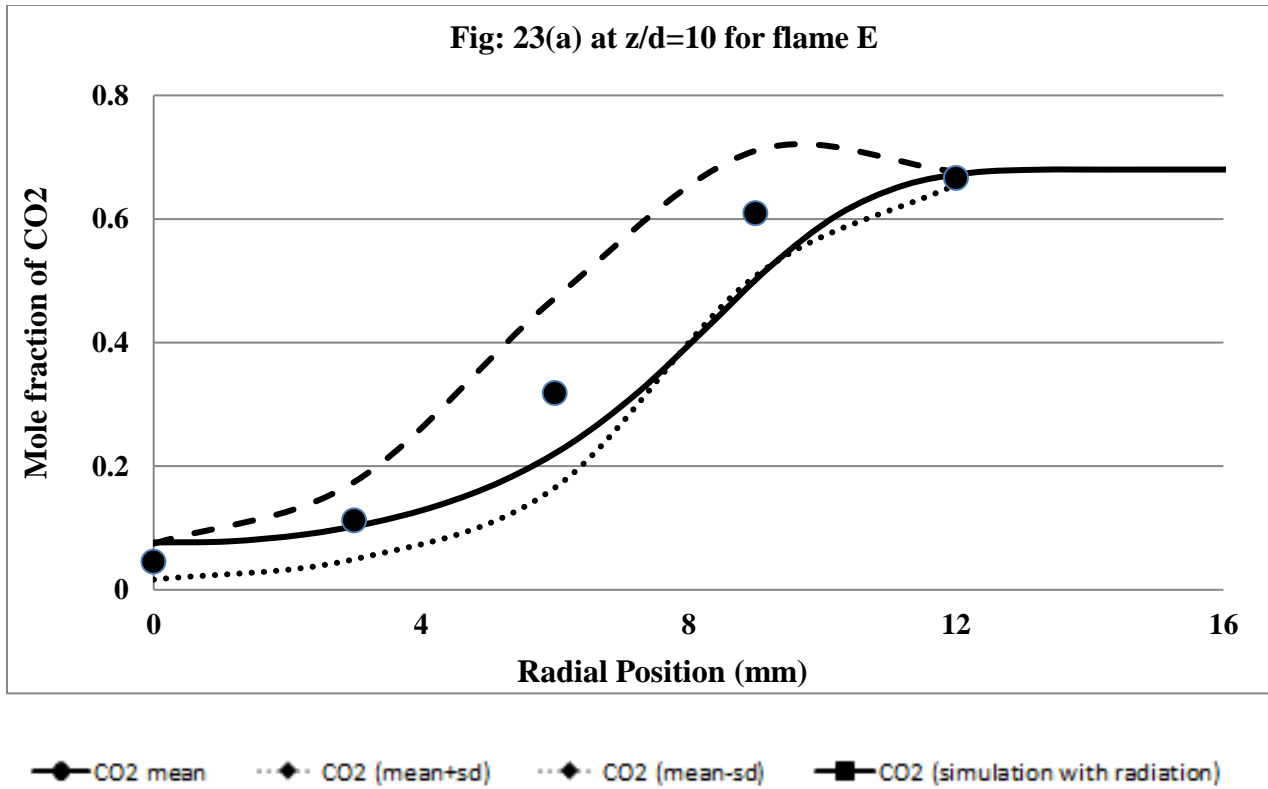


Figure 23: Radial profile distribution of CO₂ mole fraction at 50mm and 100mm height from the fuel nozzle for flame E

In the figures 25-29 below where we have plotted the temperature self-correlation versus the temperature fluctuation intensity (TFI) curves for the different flames. The coefficient of temperature self-correlation is in the range of around 12~13 (depending upon the flame conditions) with R^2 value ranging around 0.8. The deviation is due to ignoring the higher terms from equation 4. Also, though the flame conditions differ regards to Reynolds number and fuel conditions the temperature self-correlation values gave the range of around 12~13 which is almost the same. This also indicates that regardless of Reynolds number and fuel ratio for these oxy-combustion flames the turbulence radiation interaction terms do not depend upon the Reynolds number and the fuel ratio of the flames.

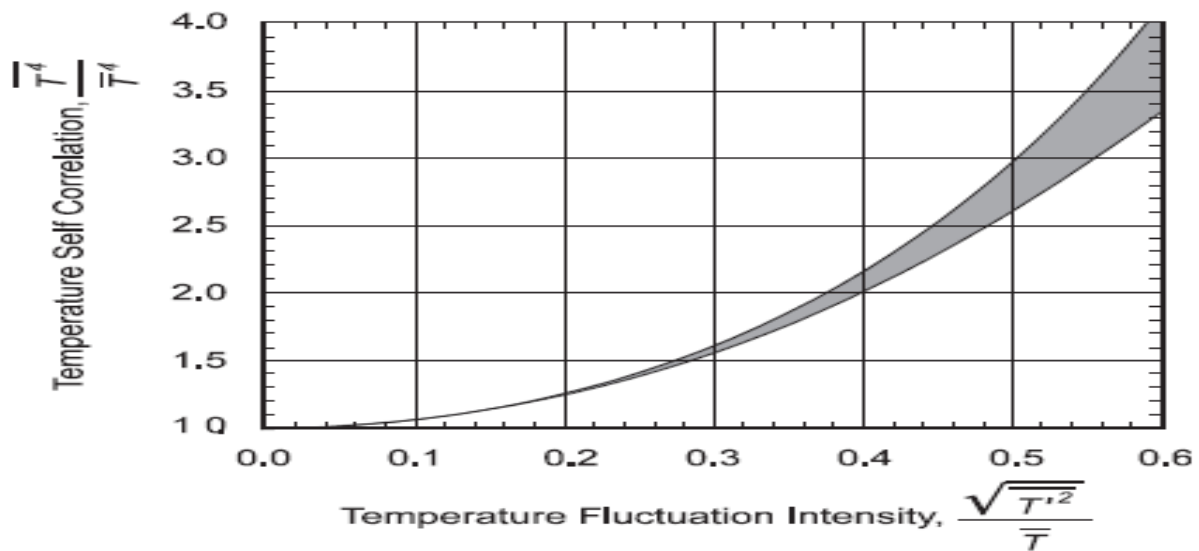


Figure 24: Temperature self-correlation as a function of the intensity of temperature fluctuations. The shaded area is the range of temperature self-correlation for the investigated pdf shapes. Adapted from [S.P. Burns, 1999]

When we take the higher order terms upto 4th order values from the figures 30-34 we see that these show good correlation values indicating good alignment with theory for the turbulent flames that we are analyzing. But we are not able to use up to 4th order in FLUENT code as they involve solving additional transport equation for these higher order moments. So our goal was to

find out from the figures 29-33 that what slope can be used that takes account of the higher orders which was the value of 12~13 in figures 29-33. These slope values were used in FLUENT code.

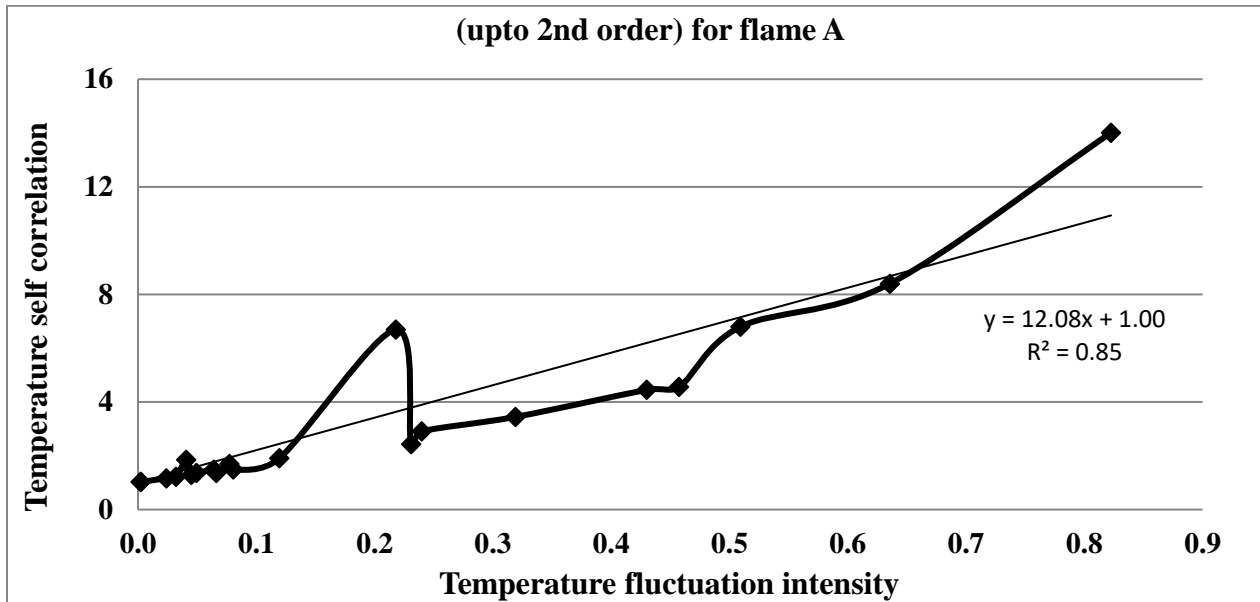


Figure 25: Temperature Self-Correlation Vs Temp Fluctuation Intensity (upto 2nd order) of flame A

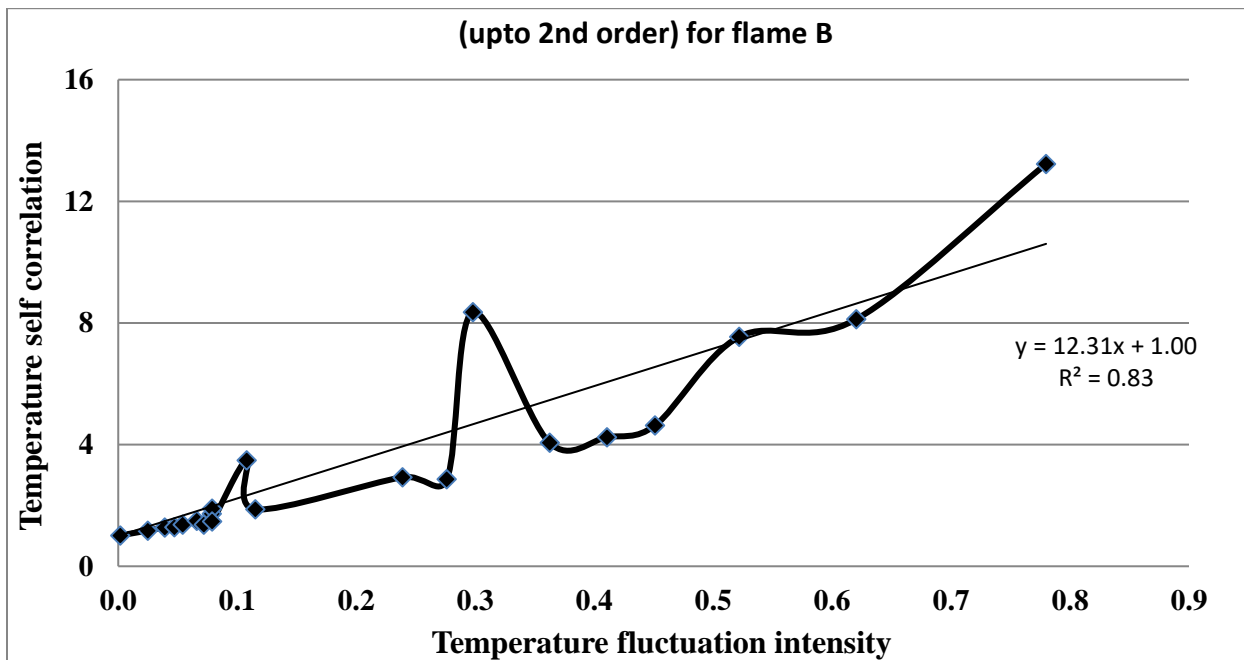


Figure 26: Temperature Self-Correlation Vs Temp Fluctuation Intensity (upto 2nd order) of flame B

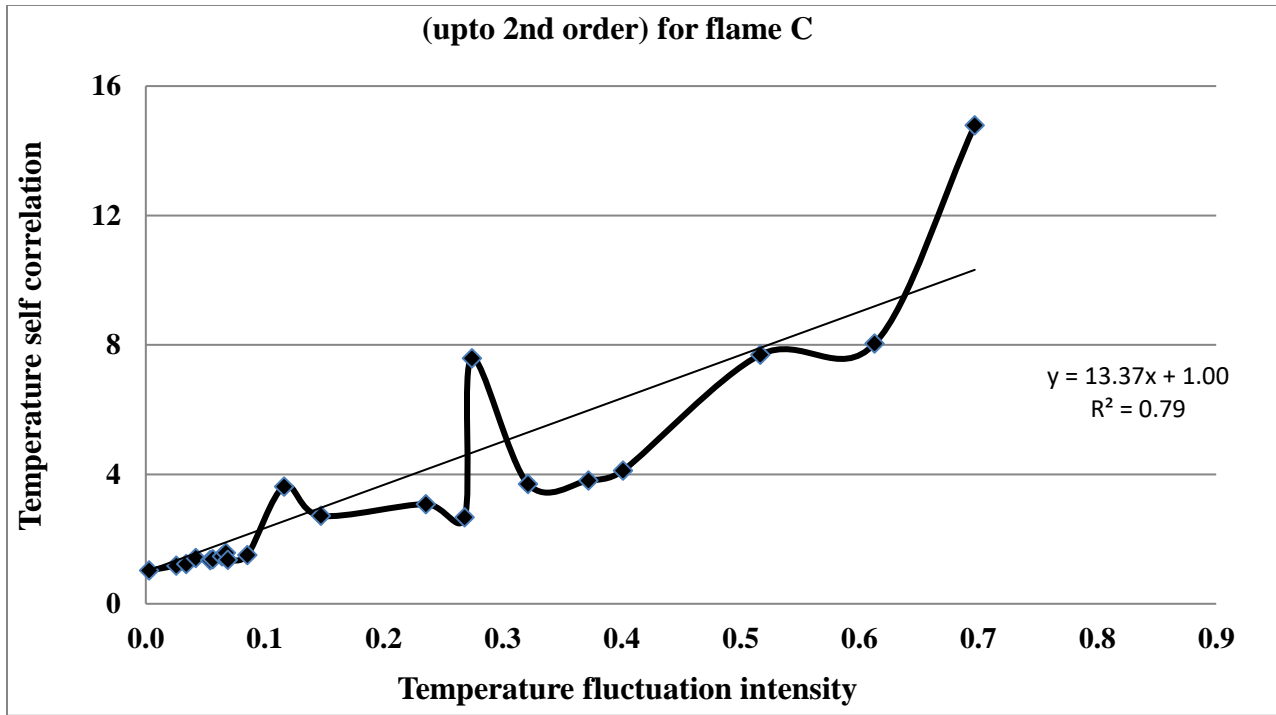


Figure 27: Temperature Self-Correlation Vs Temp Fluctuation Intensity (upto 2nd order) of flame C

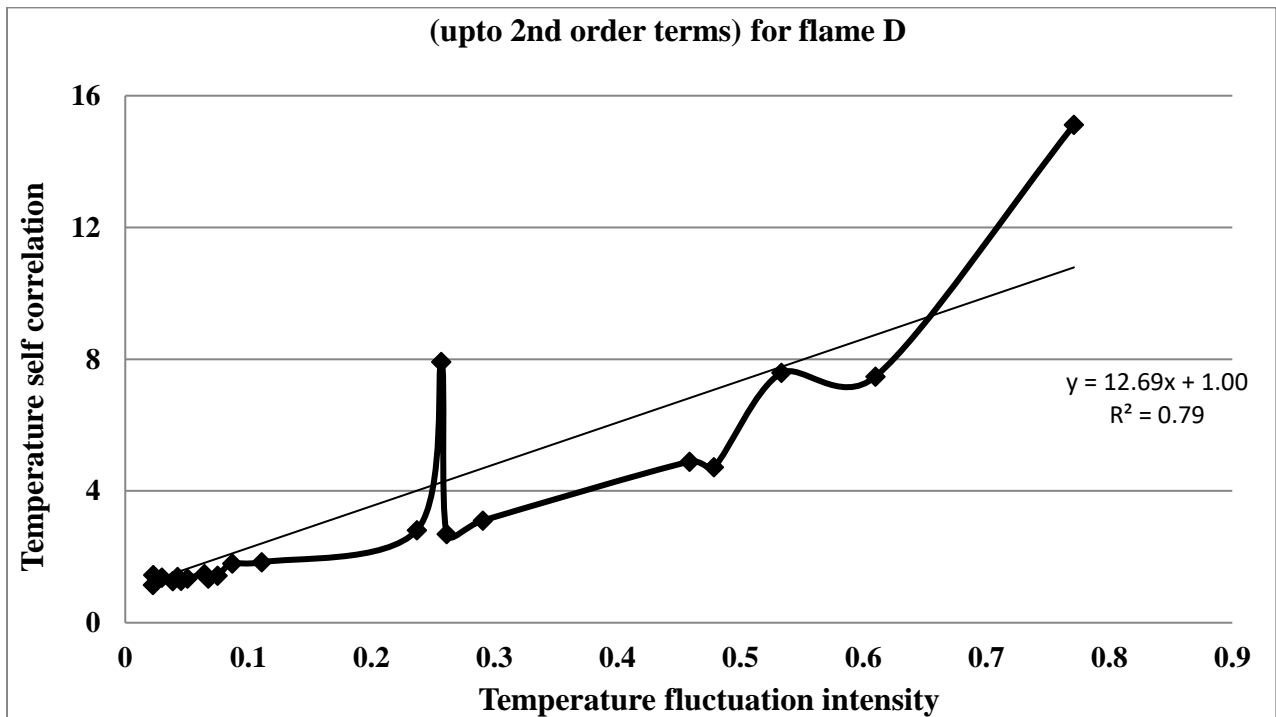


Figure 28: Temperature Self-Correlation Vs Temp Fluctuation Intensity (upto 2nd order) of flame D

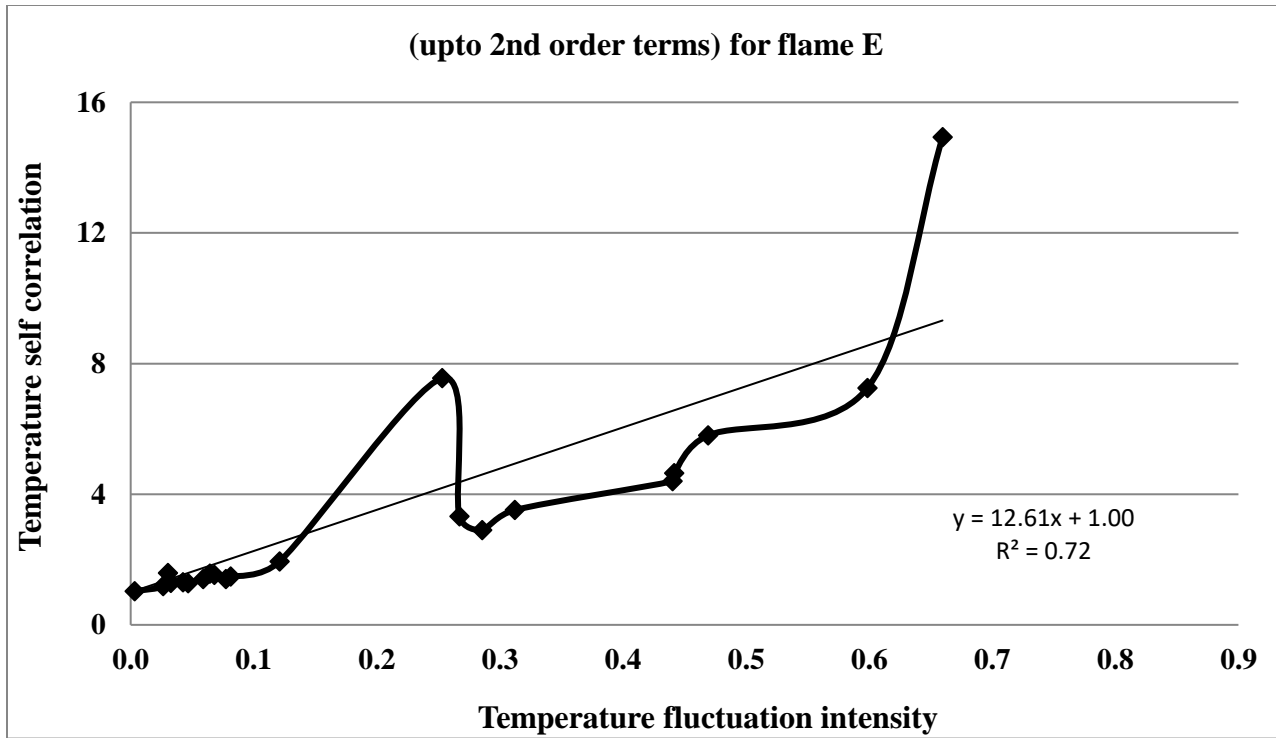


Figure 29: Temperature Self-Correlation Vs Temp Fluctuation Intensity (upto 2nd order) of flame E

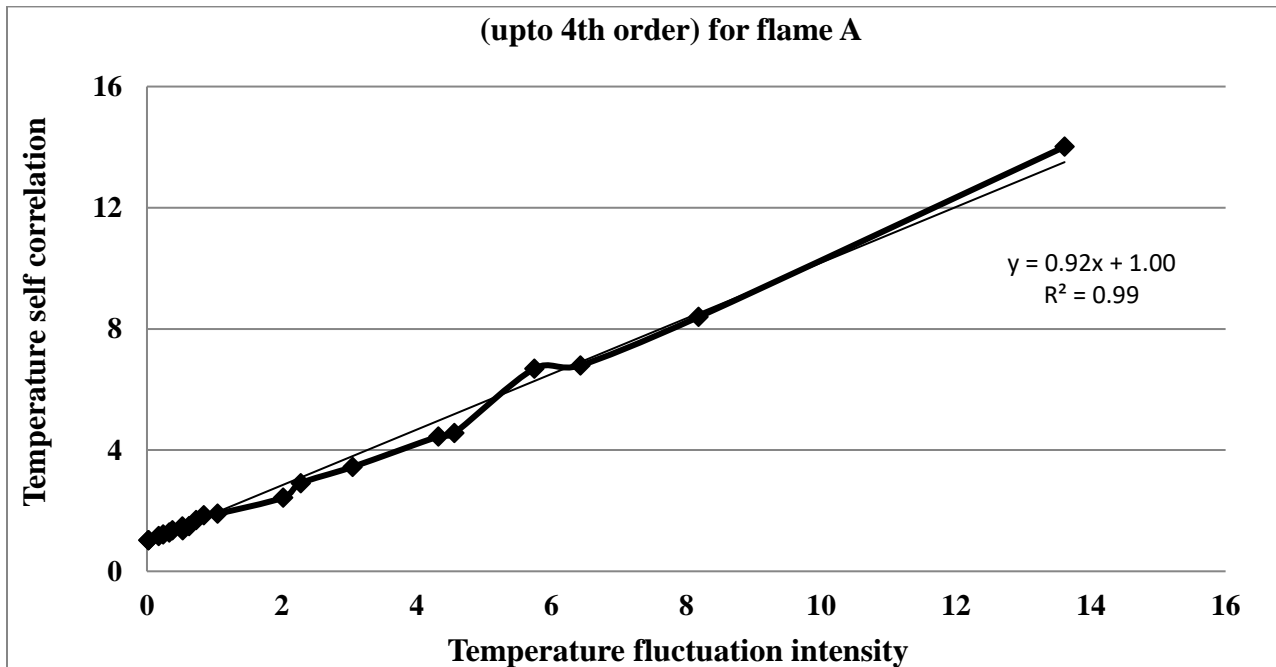


Figure 30: Temperature Self -Correlation Vs Temperature Fluctuation Intensity (upto 4th order) of flame A

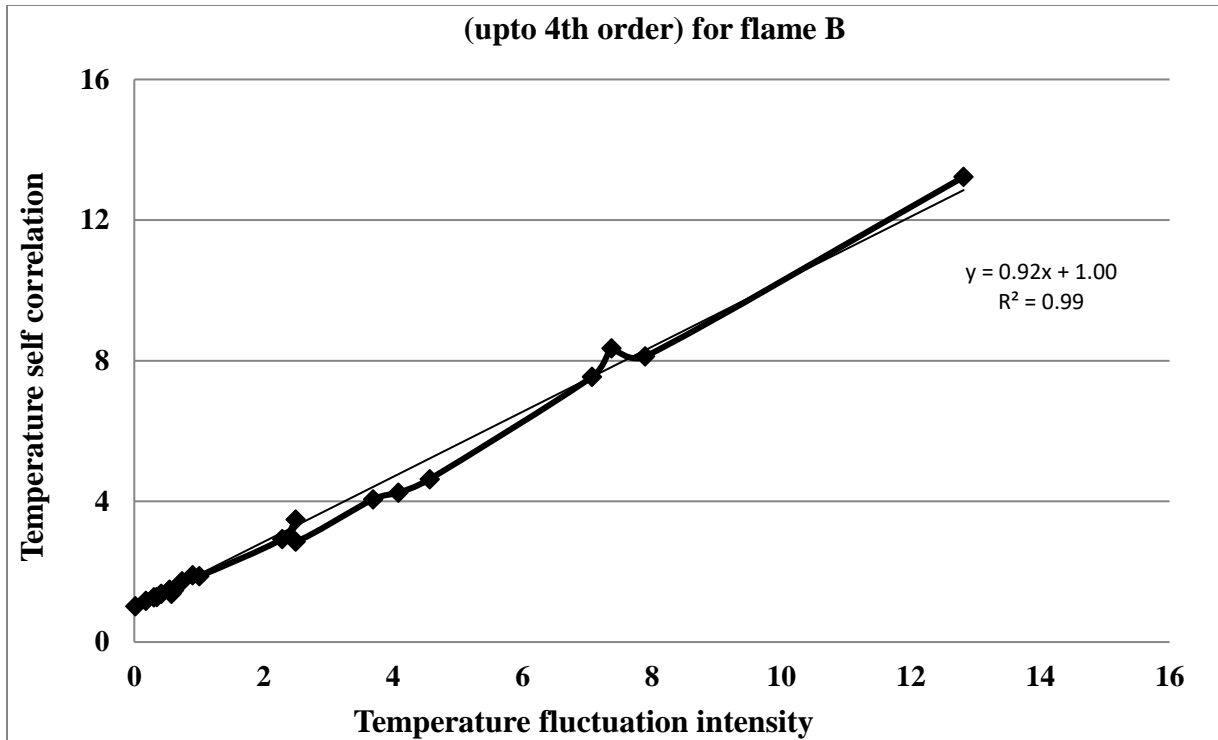


Figure 31: Temperature Self -Correlation Vs Temperature Fluctuation Intensity (upto 4th order) of flame B

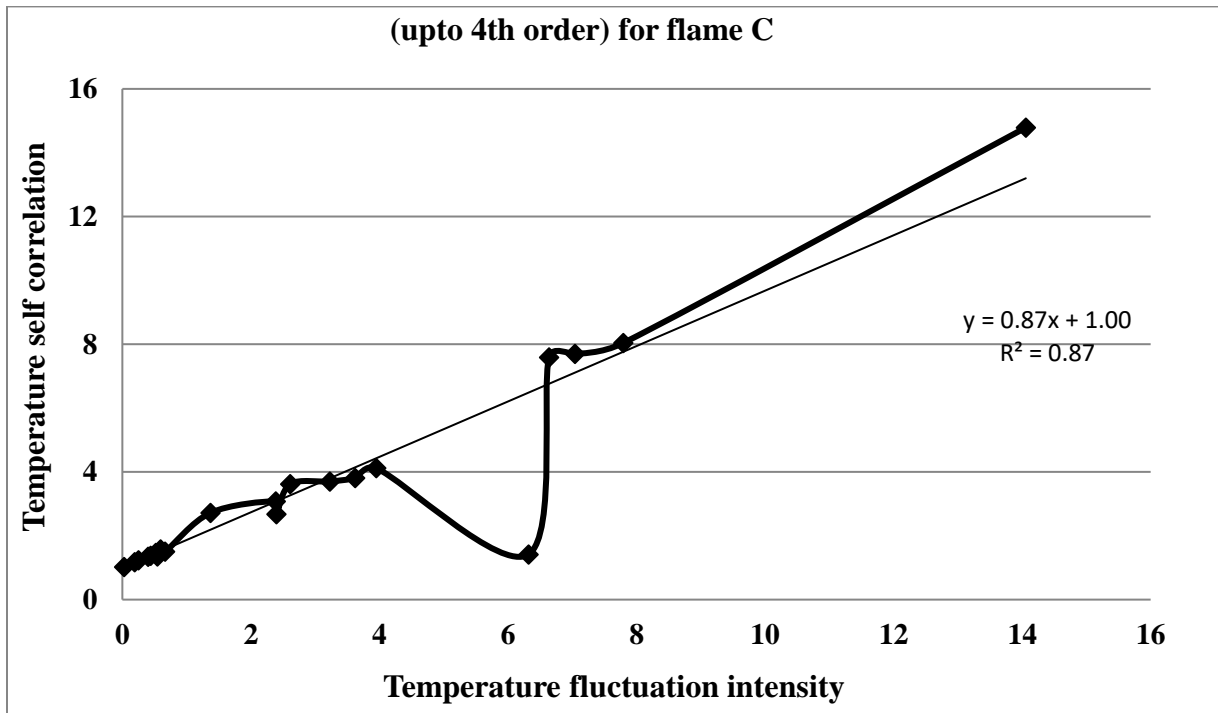


Figure 32: Temperature Self -Correlation Vs Temperature Fluctuation Intensity (upto 4th order) of flame C

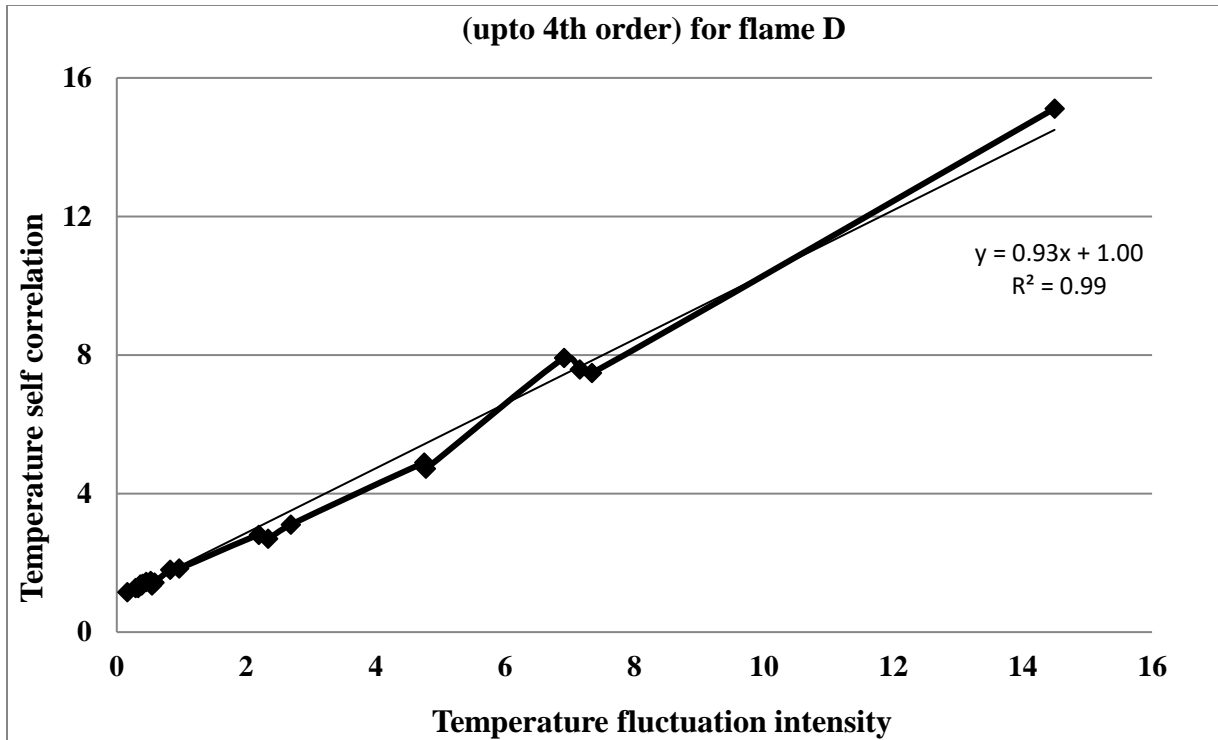


Figure 33: Temperature Self -Correlation Vs Temperature Fluctuation Intensity (upto 4th order) of flame D

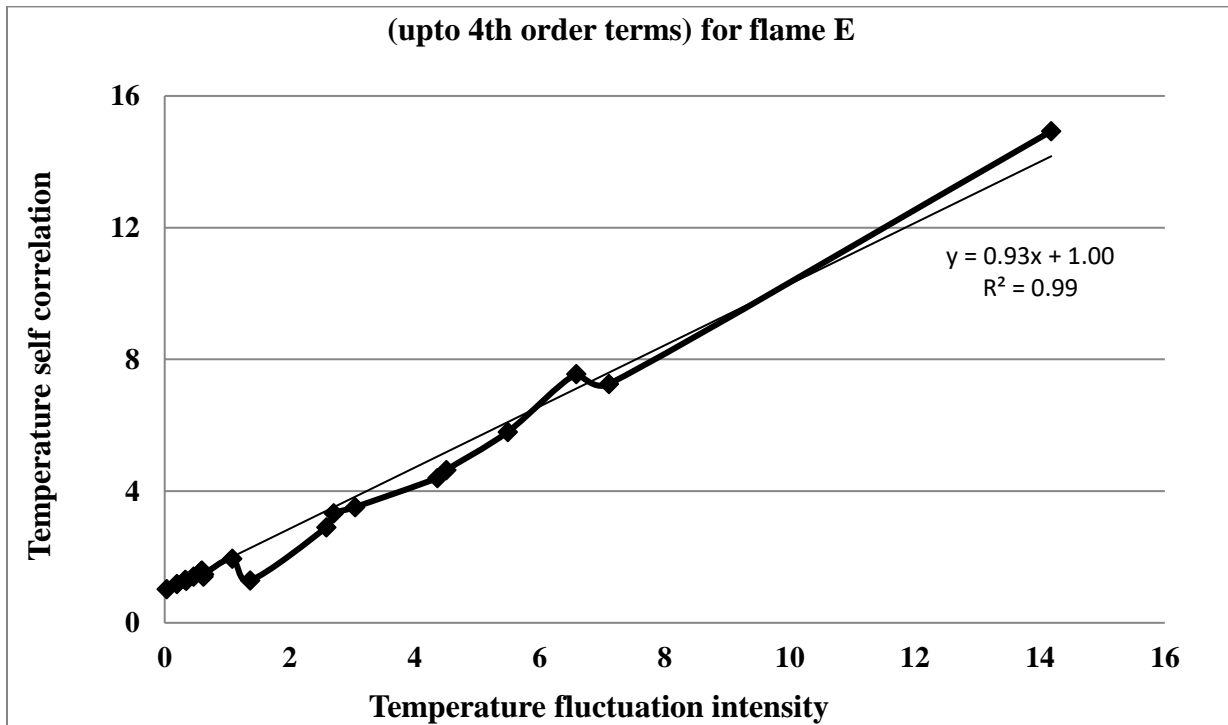


Figure 34: Temperature Self -Correlation Vs Temperature Fluctuation Intensity (upto 4th order) of flame E

Figure 35-39 shows $\overline{kI_b}$ vs $\overline{k} \overline{I_b}$ for different flames which indicates the correlation between fluctuations of the spectral absorption co-efficient and the fluctuations of Planck function which is basically the fluctuation of the temperature. The slope close to 1 (1.1) indicating that the relation between Planck function and the absorption co-efficient is not so significant for the TRI consideration at the lower region of the flame. This may occur due to the fact that fluctuation may both locally increase as well as locally decrease the concentration of H₂O and CO₂ which are the two most participating gases in combustion systems [14]. Fluctuation locally increasing the concentration of the species implies the greater conversion of reactants into products that corresponds to local increase of temperature and the vice versa for locally decreasing of concentration. These two affects each other to almost nullify the overall effect of absorption co-efficient and Planck function on TRI.

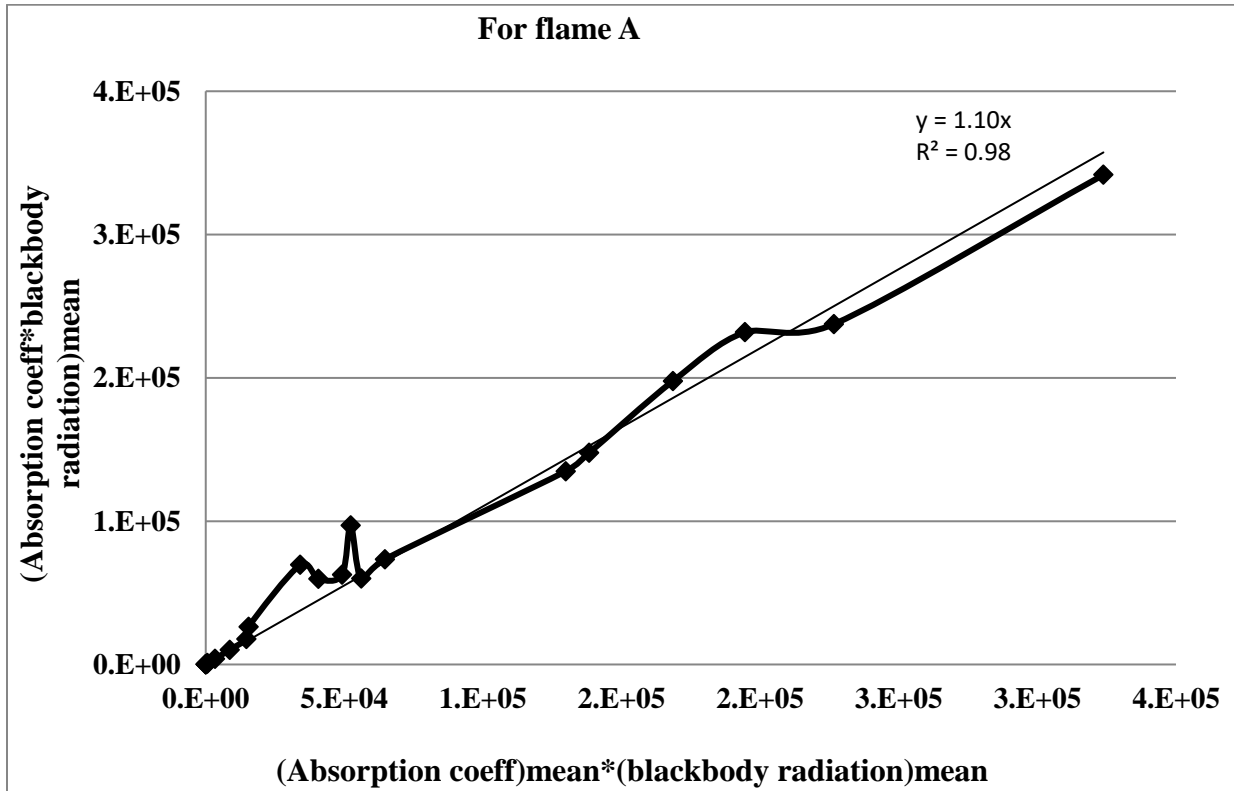


Figure 35: (K**I**)whole mean vs Kmean*Ibmean for flame A

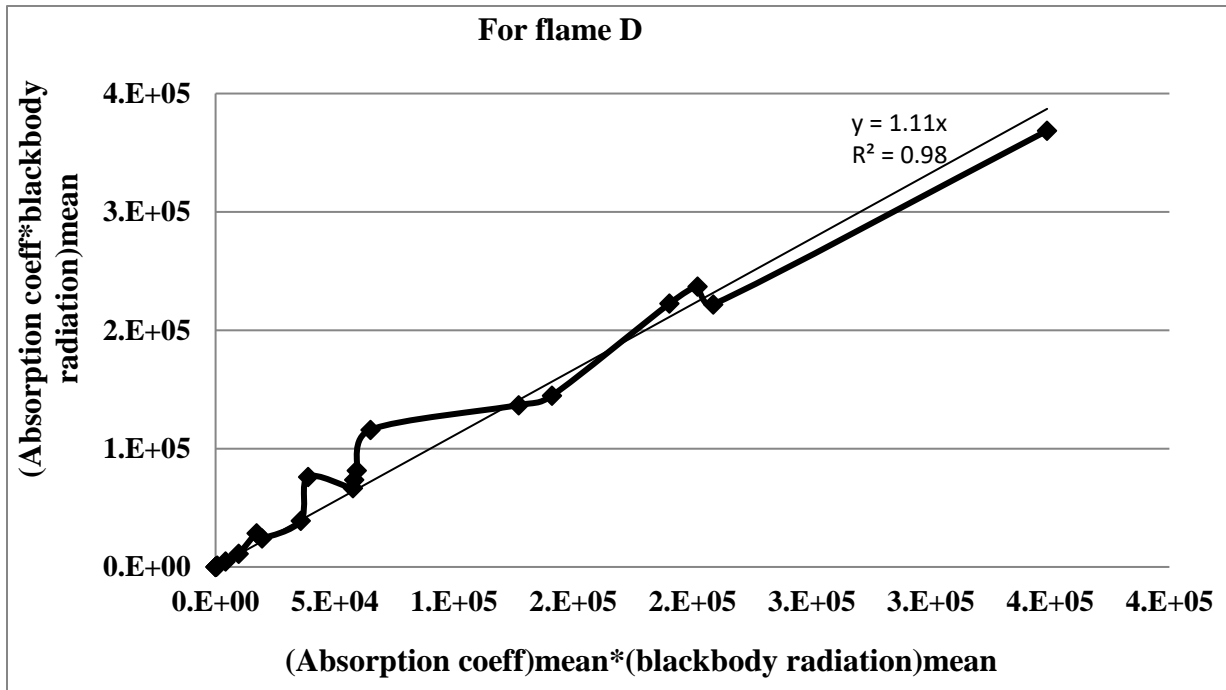


Figure 38: (KIb)whole mean vs Kmean*Ibmean for flame D

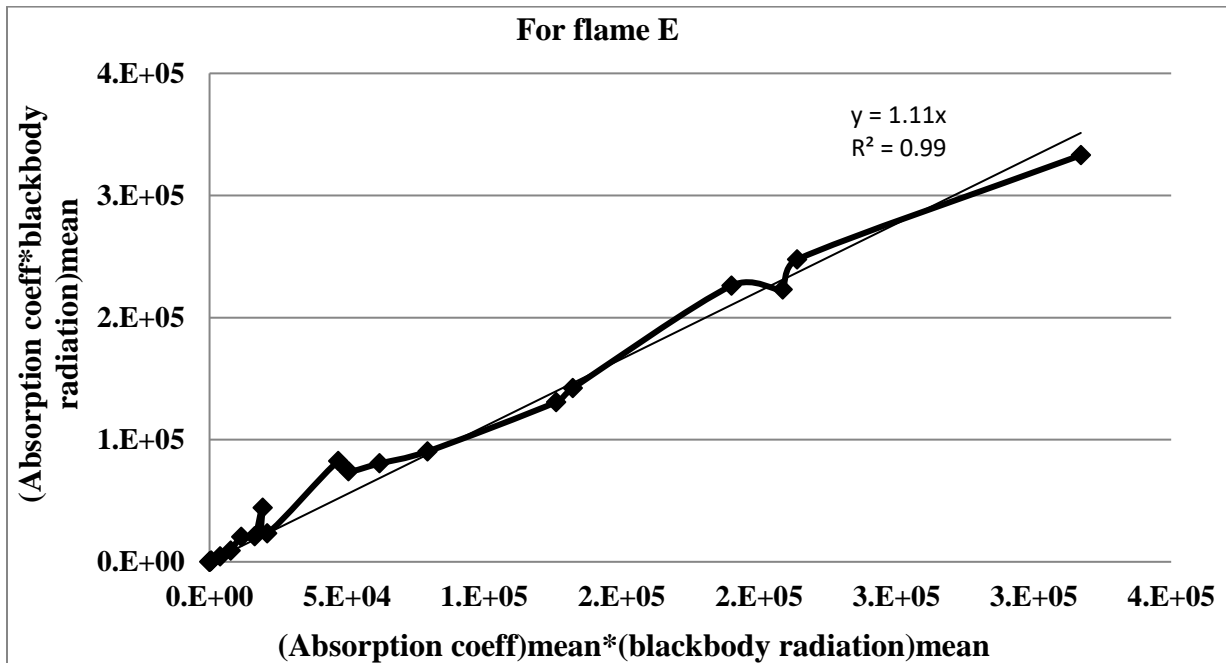


Figure 39: (KIb)whole mean vs Kmean*Ibmean for flame E

The modeling with the results of TRI analysis was done using UDF having the slope as 12 for the temperature self-correlation equation. The modeling was used in flame D. The radiation amount from the simulation was found by using a scheme file and clipping the flame region using the same CO mole fraction as described previously. Finding the mass flow rate of the fuel mixture from the FLUENT and knowing the theoretical heat combustion value of the fuel we can calculate the radiant fraction value from FLUENT.

Flame modeling	Total heat transfer rate in Watts	Radiated heat transfer in Watts	Radiant fraction (%)	% increase in radiation for TRI inclusion
Without TRI	17241	1424	8.26	73.49
With TRI	17241	2471	14.33	

Table 4: Results of flame D for TRI inclusion

CHAPTER V

CONCLUSIONS

Conclusion

Most simulations of turbulent combustion systems reported in the literature, employ the Reynolds Averaged Navier Stokes (RANS) framework. Here, a time-averaged representation of the flame field is obtained during the solution process. However, the variables of interest to radiative transfer have non-linear dependencies on the flame field. Therefore, using time-averaged variable values in the radiation calculations can result in incorrect answers. The goal of this study was to improve the fidelities of the radiation calculations by formulating Turbulence-Radiation Interaction (TRI) models using experimentally measured data.

This thesis utilizes experimental measurements from five highly turbulent oxy-methane flames ($\text{CH}_4/\text{H}_2\text{-O}_2/\text{CO}_2$) of varying Reynolds numbers and fuel composition carried out at Sandia National Laboratories. RANS simulations of these turbulent flames were first carried out. The numerical time-averaged predictions agreed well with the mean flame measurements of temperature, specie field along several radial and axial locations, providing credibility to our modeling technique. The root mean square temperature (T_{rms}) which is a critical variable for formulating TRI models also agreed well with experimental measurements. The computed T_{rms} value was then employed to compute the enhancement in the emission term due to temperature fluctuations by formulating a model for the enhancement factor using experimentally measured temperature fluctuation data. The validity of the model and the statistical analysis of the data was established through a Taylor's series expansion of the Planck's blackbody emission term.

Accounting for this enhancement in the emission term increased the radiative flux predictions by 70% across all flames. The study shows that it is important to account for TRI models in CFD simulations or else the heat fluxes to the wall may be under-estimated.

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