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SIMULATION OF AN ETHYLENE FLAME WITH TURBULENCE, SOOT AND RADIATION MODELING

BY

SANTU GOLDER

A thesis submitted in partial fulfillment of the requirements for the

Master of Science

Major in Mechanical Engineering

South Dakota State University

2018

SIMULATION OF AN ETHYLENE FLAME WITH TURBULENCE, SOOT AND RADIATION MODELING

This thesis is approved as a creditable and independent investigation by a candidate for the Master of Science in Mechanical Engineering degree and is acceptable for meeting the thesis requirements for this degree. Acceptance of this does not imply that the conclusions reached by the candidates are necessarily the conclusions of the major department.

Jeffrey Dbom, Ph.D.
Thesis Advisor Date

Kurt Bassett, Ph.D.
Head, Department of Mechanical Engineering Date

Dean, Graduate School Date

I DEDICATE MY THESIS TO MY PARENTS.

“ The future belongs to those who believe in the beauty of their dreams.”

Eleanor Roosevelt

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At first, I would like to thank my adviser Dr. Jeffrey Doom for giving me an opportunity to work on combustion. His invaluable guidance and advise helped me to complete my thesis. His intelligence, patience and experience was influential. I am very grateful for his great graduate support. It has been a great pleasure working Research High Performance Computer Specialist Brian Moore. I thank them for stimulating discussions and for sharing their time and insights with me.

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I am also very grateful to my father Sujit Golder and mother Saraswati Golder for their incredible patience and generous support. I would like to thank to my brother Sourav Golder for bringing joy and happiness in my life. Finally, I would like to thank to the professors and student of Mechanical Engineering department for providing a wonderful place to study and work.

”Be patience and work steady” this is the most important advice that my father taught me.

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ABSTRACT

SIMULATION OF AN ETHYLENE FLAME WITH TURBULENCE, SOOT AND RADIATION MODELING

SANTU GOLDER

2018

This thesis will investigate soot models that are available in commercial codes. We will look at the effect of turbulence models, gravity, soot models and radiation. Simulations will be compared to Coppalle and Joyeux [1]. The flame is an ethylene air diffusion flame at a Reynolds number of 5700. Simulations show the SST turbulence model, one-step soot model and Rosseland radiation model including gravity agree well with experimental data (temperature and soot). Flamelet soot modeling from Carbonell et al. [2] and flamelet radiation modeling from Doom [3] has been incorporated and compared as well.

1 INTRODUCTION

In this modern age, people are highly dependent on fossil fuels. Petroleum based combustion leads to several kinds of pollutants (e.g. NO_X, SO_X, CO, hydro-carbons and particle matter). Particle matter named ”soot” is a well-known carcinogen and odorous pollutant.

Combustion benefits us. Also combustion affects our society negatively by generating environmental pollutants such as oxides of nitrogen and greenhouse gas. It is more and more critical to obtain combustion process of high fuel efficiency but lower pollutants considering the importance of combustion and lowering the resources of fossil fuels. Most combustion processes arise in a turbulent flow environment such as automobile engines, gas turbine combustors and industrial burners. Turbulence combustion is the most challenging subject in the engineering sciences that includes complex physical and chemical phenomena which interact strongly with one another.

Until almost 30 years ago, the combustion technology depends almost on experimental methods. Providing the most realistic answers to many combustion, experimental method suffers from scaling problems, measurements difficulties, operating costs, and the time [4]. In comparison with the experimental method numerical modeling is less expensive and take less time. Also they can provide very important information as well.

Soot the good, the bad affects life in many ways. Soot is mainly carbon named char produced at high temperature during combustion of fossil fuel or in a pyrolysis process. A complete soot model include both soot formation and oxidation. At first fuel molecule are separated into smaller hydrocarbon molecules and free radicals for both combustion and pyrolysis system.

The aromatic species grow with the addition of other aromatic and smaller alkyl species to form Poly aromatic hydrocarbon. The growth of PAH leads to smallest identifiable soot particles with diameter of 1 nm and with masses of around 1000 amu [5].

The soot particle are in spherical shape and have Carbon , Hydrogen ratio. Soot particles coalesce into larger spherical particles and then undergo surface reactions with surrounding gaseous species, dehydrogenate, oxidize and coagulate. Soot that is produced during combustion typically has C/H ratio of 10 and aggregate structure [6].

Production of soot particles in a flame is a chemically-controlled phenomenon. Gaseous molecular hydrocarbon are converted to solid carbon formed to soot. Thus thermodynamics can't explain the details process of soot production. So the chemical kinetics play very important role for soot production.

Detailed chemical mechanisms are required to explain combustion simulation such as ignition, pollutant emissions, soot, CO and unburned hydrocarbons. Radiative heat transfer needs to be considered in combustion simulation because the influential heat transfer mode due to its dependence on temperature [7]. Radiation changes the flame temperature that affects the flow field and changes the density and affects the pollutant emission [8]. Soot is a major pollutants and the formation of soot represents the incomplete combustion.

Carbon black is used every where in our daily life. It is mainly used as reinforcing agent in rubber products as tires, tubes, cables and other mechanical rubber goods. Carbon black is also used as black pigment in printing, carbon paper, typewriter ribbon inks, paints, plastics, fibers and ceramics; also in leather finishers, manufacturer dry-cell batteries, electrodes and carbon brushes, conductive and anti static rubber and plastic products, video disks and tapes and also widely used in high temperature insulating material.

With the advancements of physical understanding of numerical method with chemical mechanisms and radiation model, combustion modeling is becoming more and

more knowledgeable. A complete combustion simulation should be capable of providing detailed information of properties such as pressure distributions, velocity fields, chemical species compositions, pollutants formation, radiative heat loss and so on.

Soot formation and thermal radiation are closely coupled factors in determining flame structure, temperature and pollutants emissions and have particular significance in ox-fuel combustion. Industrial oxy-fuel have low momentum, highly luminous flames [9]. In glass melting industries oxy-fuel burners are very useful [10].

In diesel engines, gas turbine combustors and industrial burners non premixed combustion process is occurred. In the non-premixed combustion process fuel stream and oxidizer stream are initially separated and when the two stream mixed with each other, at that time non-premixed flame formed.

On the contrary, soot contributes to many serious problems for contribution of pollution. Soot enhances the emission of other pollutants from flames (i.e. carbon-dioxide, carbon monoxide, nitrogen oxide). Soot emits radiative heat from combustion chamber that causes unwanted fire and hampers fire fighting efforts.

Particle matter named ”soot” is a well-known carcinogen and odorous pollutant. Particle matter can penetrate into respiratory tracts and cause health problems [11]. During takeoff and climbing operation mode, soot emissions are at the highest modes and it increases the risk of cancer, respiratory and cardiovascular diseases for people living near an airport [12]. Environmental Protection Agency (EPA) is setting stricter emissions on soot because soot absorbs solar radiation in the atmosphere and act as vapor condensation nuclei [13].

Practical combustion devices of gas turbines are mostly designed based on experimental findings, which are expensive for high quality test. Besides the experiments, numerical simulations are useful approach that can improve the combustion emission of these harmful pollutants and are useful tool for engineers. Therefore, the need for better soot models and the understanding of current modeling on soot emissions (including radiation) are imperative.

For complete combustion three things are necessary: Oxidizers, Fuels and Ignition sources. There are three types of Oxidizer such as Liquid, Gases and Solids. Oxygen, fluorine, chlorine, hydrogen peroxide, nitric acid, per chloric acid are gaseous oxidizers. Fuels are three types also. Gasoline, acetone, ether, Pentane are liquid fuel, Plastics, wood, dust fibers are solids and acetylene, propane, carbon monoxide, hydrogen are gaseous fuels. Only fuels and oxidizers can't bring fire. Finally for creating fire needs to be an ignition source. Sparks, flames and static electricity heat are the ignition sources. Finally, combining Oxidizers, Fuels and Ignition sources fire can be found. The Complete combustion can be defined by the figure 1. [14]

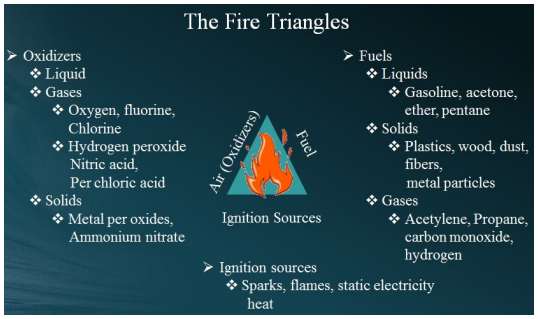


Figure 1: Fire Triangle.

Figure 2 [15] shows main parts of jet engine. At first, fresh air is sucked and compressed in low pressure compressor. Compressed air is then compressed in high pressure compressor. In the combustion chamber compressed air mixed with fuel and burner helps for ignition. The high pressure gas passed through high pressure turbine and low pressure turbine and move out from the nozzle. In the combustion chamber, combustion is turbulent. Navier-Stokes equations solves the combustion problem. Reynolds Average Navier-Stokes (RANS) Simulation, Large Eddy Simulation predict the combustion phenomena such as Soot, NO_x, Hydrocarbon and so on.

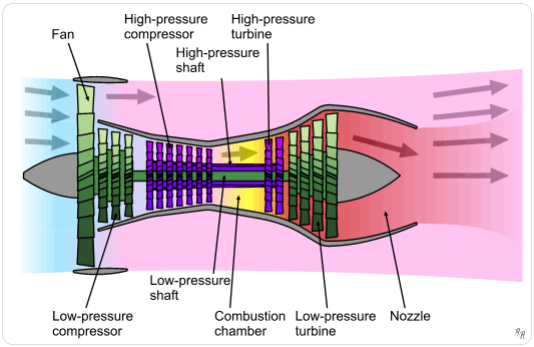


Figure 2: Jet Engine parts.

One of the simplest model of jet engine is modeled in CATIA V5 shown in figure 3.

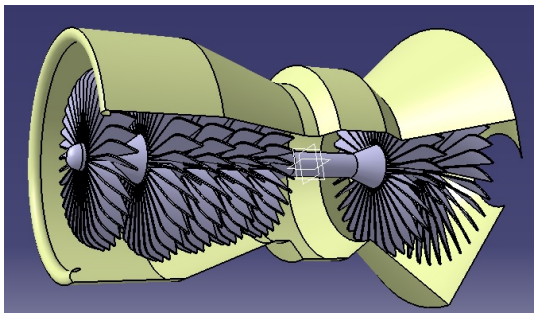


Figure 3: Jet Engine.

Figure 4 [16] shows the main parts of Internal Combustion engine for spark ignition system. According to Internal combustion Engine Wikipedia during intake valve is opened, the piston goes to Bottom Dead Center (BDC) and fresh air and fuel mixture is taken inside the cylinder. After that intake valve is closed and the mixture is compressed. With the help of spark plug of air-fuel mixture is then burnt in Top Dead Center (TDC). The working strokes is started and piston goes to Bottom Dead Center (BDC) again. At that time exhaust valve is opened and exhaust gas goes out. In internal combustion engine burning is also turbulent. This combustion is also computed by Reynolds Average Navier-Stokes (RANS) Simulation, Large Eddy simulation.

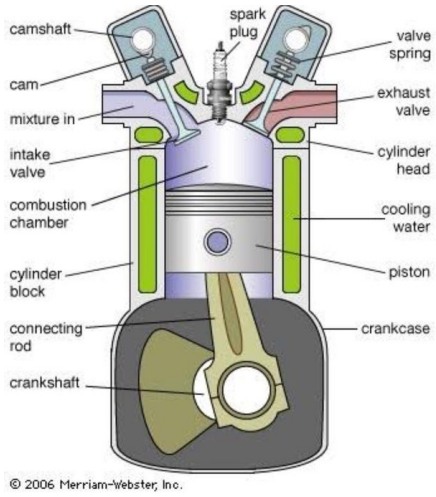
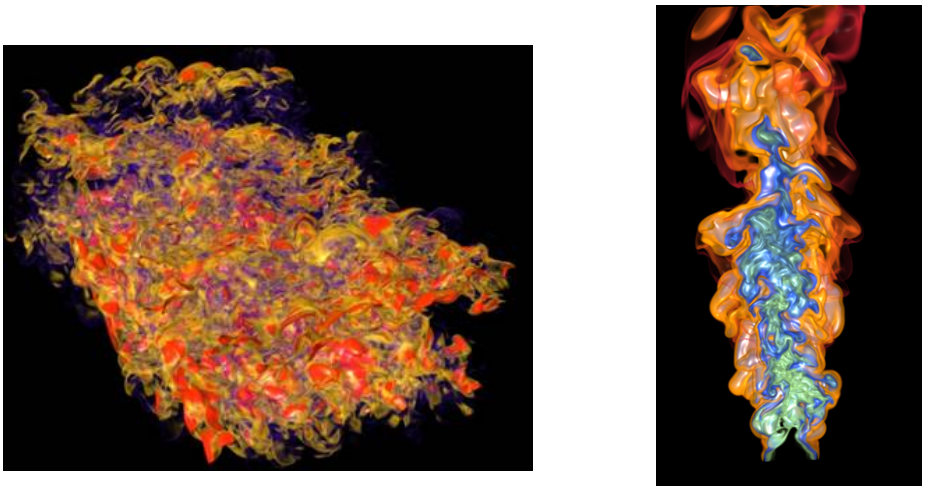


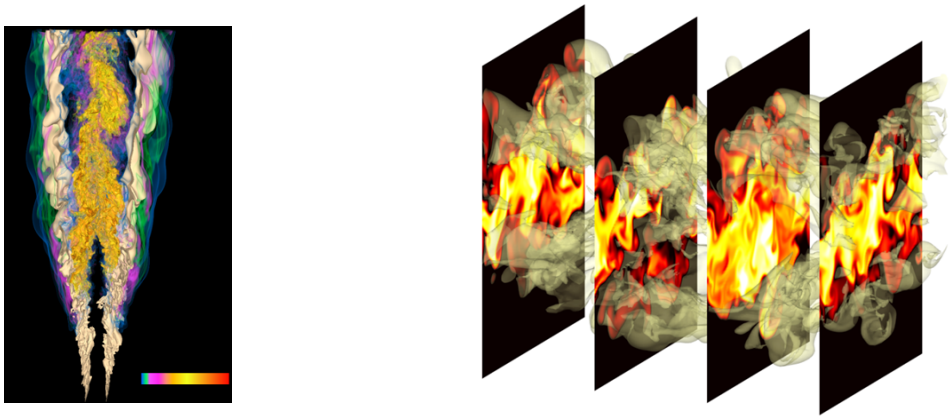
Figure 4: Internal Combustion Engine.

DNS explains the possibilities of performing of full simulation for developing turbulent combustion in grid. In terms of scalar dissipation for reaction chemistry mechanism, the DNS data are very useful for developing turbulent mixing reaction simulation. There are some predictions of direct numerical simulation (DNS). Firstly, how do the detailed transport and chemistry affect the mixing rates in reactions. Secondly, how do the reduced parameterizations of the thermo-chemical state can be explored [17]. Figure 5 and 6 [18] are most recent Direct Numerical Simulation (DNS).



5 (a) 5 (b)

Figure 5: 5 (a) Ethylene no-premixed flames with 350 M grid points. and 5 (b) Lean premixed flames 200 M grid points.



6 (a) 6 (b)

Figure 6: 6 (a) Lifted flames with 1 B grid point. and 6 (b) CO/H2 Non-premixed flames with 500 m grid points.

1.1 OVERVIEW

British Chemist Sir Humphry Davy firstly started the combustion Chemistry from 1813 to 1815 based on Gas explosions in coal mine. This field is also defined as Davy's discoveries. He also discovered the catalytic combustion. [19]

In 1970 countries were experiencing energy crisis, then combustion research started to minimize consumption of fossil. Long lines at the gas pump caused the nation to prioritize toward reducing the dependence on imported oil for developing energy efficient automobiles. [20]

Beginning of combustion research, automotive engineers did not have laser and supercomputers for getting deep knowledge on combustion. Researchers from Sandia and other national laboratories realized the complexities of combustion research. Comprehensive and skilled knowledge of combustion process can improve the combustion research.

Technology is developed now and researchers are using laser, mirror and super computer tools to investigate turbulent reaction flow. Also researchers from Sandia national laboratory found hyper sonic and supersonic jet propulsion system during the designing of weapon component. Raman spectroscopy was used to identify the chemical species within a gas. When scattered beam is passed through a flame researchers can examine the chemical composition of combustion flame.

In 1973 Bob Setchell, and Taz Bramlette, Hartley proposed for combustion research at Sandia to the Atomic Energy Commission, which later became Energy Research and Development Administration and then the Department of Energy. Proposal was expanded to national center for combustion research. It took several years for gaining support and approval. Finally, in 1980 combustion research facility (CRF) opened to researchers and Hartley was first director. Combustion center one of Sandia's first user facilities located outside fences and classified weapon development areas. The research program welcomed researchers from industry and universities. CRF conducts work with

university and researchers and provides opportunities for university postgraduate research. Combustion research facility (CRF) researchers expanded the combustion processes and contributed to significant design revolutions for diesel engines, pulse combustors for furnaces and pollution reduction methods. [21]

Researchers are now moving towards numerical combustion research. Numerical results are also compared with experimental results that gives verification of numerical simulation. Numerical simulation is cheap and easy to apply. There are lots of commercial software such as ANSYS, CHEMKIN, Star CCM, Comsol. OpenFOAM is a noncommercial open source software. Reaction mechanism helps to predict combustion products such as soot, carbon dioxide, nitrogen oxide, hydroxide, hydrogen peroxide can be predicted. Researchers are now modifying Naiver-Stokes equations for getting better results. Direct Numerical Simulation (DNS) is advanced research. Now researchers are working for development of DNS combustion.

Experimental combustion research technique is changing day by day. Burner stabilization is changing too. Burner is implementing for both premixed and non-premixed combustion and also burner is implementing in high and low pressure condition.

Following are the most recent experimental combustion research

- Low-temperature combustion
- Dilute (or lean-burn) gasoline combustion
- Clean diesel combustion

Low temperature combustion is flameless, staged burning of the fuel at low temperature, for dilute gasoline combustion, flame moves through either premixed or non-premixed mixtures of fuel and air. In clean diesel combustion, fuel-air mixing occurs prior to the flame produces less soot as well as improves efficiency of engines. [22]

1.2 LITERATURE REVIEW

Particle matter can penetrate into respiratory tracts and cause health problems [11]. During takeoff and climbing operation mode, soot emissions are at the highest modes and it increases the risk of cancer, respiratory and cardiovascular diseases for people living near an airport [12]. Environmental Protection Agency (EPA) is setting stricter emissions on soot because soot absorbs solar radiation in the atmosphere and act as vapor condensation nuclei [13].

There are various reasons to accounts for soot formation in flame [23]. Soot presents in commercial aircraft's exhaust gases. For the nucleation of cirrus clouds, this exhaust gas is suspected [24]. Soot particle are desirable but unwanted at the outlet of industrial furnace or boilers where heat exchange is maximized through radiation [25]. For the designer it is a challenge which will be overcome with the predictions of soot formation. It can be said that acetylene is a precursor for soot formation [26]. According to Kennedy [27], soot formation and oxidation models are classified in order of growing complexity as empirical, semi-empirical and detailed models.

Takahashi and Glassman [28] showed the particle formation is a correlation of pressure, equivalence ratio of unburned gases, and temperature for premixed flame. These correlations were specifically developed to predict soot formation in gas turbines and diesel engines. Frenklach and Lawrence [29] modeled the coalescence and aggregation of two soot particles. Harris and Maricq [30] discussed the role of fragmentation in defining the size distribution of diesel soot. According to Hydrogen Abstraction Carbon Addition (HACA) the most recognized pathway of acetylene addition to a soot particle is free radical mechanism.

Mueller et al. [31] found that soot formation and growth are strongly affected by turbulence. Antonio Attili et al. [32] described soot nucleates mainly in layers close to flame and spreads on the rich side of the flame due to the fluctuating mixing field. The results also show the leading order effects of turbulent mixing in controlling the dynamics

of soot in turbulent flames. Bisetti et al [33] stated soot drifts in mixture fraction space due to it's high Schmidt number and significantly lower mass diffusivity compared to gas phase scalars.

The oxidation of soot particles plays an important role in soot particle dynamics. Jean-Louis Consalvi [34] found that for methane, the soot production increases and decreases linearly with the molar concentration. Specially in higher surface area results in higher surface growth and condensation rates. Mehta and Das [35] solved for exhaust soot concentration in diesel engines using an empirical soot model. Harris and Kennedy [5] and Young and Moss [36] solved for soot volume fraction and particle number density in laminar and turbulent ethylene-air diffusion flames respectively using semi-empirical soot models. Lindstedt [37] simulated laminar flames of soot for counter flow and co-flow flames. Kee et al. [6] simulated premixed and diffusion flames.

Soot enhances the heat fluxes in furnaces [25]. In the combustion chamber of an aircraft engine soot affects the thermal balance and the gases temperature seen by the turbine blades, where life expectancy is a key issue for engine manufacturers where blades can also be physically damaged by soot particle collisions. For jet flames, soot was modeled by a sectional approach [38], which is the most complex formalisms and in simpler way, with a semi-empirical model [39].

Pistch et al. [40] applied unsteady flamelet modeling for soot formation in a turbulent methane/air jet diffusion flame where a kinetic based soot model is used. Claramunt et al [41] investigated the laminar flamelet concept to multidimensional numerical simulation of non-premixed laminar flames. They studied lagrangian flamelet for unsteady and differential diffusion with constant Lewis number.

To describe the formation of soot precursors, various levels of modeling were investigated. Sectional methods gave satisfaction to describe PAH chemistry. Zamuner and Dupoirieux [42] and recently Di Domenico et al. [43] used one along with a PAH-based soot formation model to compute laminar flames and a turbulent one [42],

with the aim of applying this approach to gas turbine simulation. However, the PAH formation route remains computationally expensive to describe. Empirical soot models were developed to obtain a strong decrease of calculation cost. They are based on correlations resulting from experimental measurements. They only depend on mixture fraction [44, 45] or fuel concentration [46, 47] and some of them use an intermediate species to model the role of soot precursors i.e. to decorrelate soot formation and fuel oxidation [47, 48]. Computational cost is low and attractive but they are inherently not predictive and conditions of use are limited.

1.3 ORGANIZATION OF THE WORK

The paper is organized as follows. The following section is a discussion of turbulence models and soot models that are used in this study. Next section is the results of the different soot models. Also, the effect of gravity and radiation has been discussed for the flame propagation and NO_X formation. Finally, the two-equation soot flamelet model from Carbonell et al.[2] and the flamelet radiation model from Doom [3] has been included to look at soot formation. The last section is a brief conclusion.

1.4 CONTRIBUTIONS

The Principle contribution of this works are:

- This thesis described the reasonable model for predicting temperature and soot formation for RANS model considering different Soot model with the effect of radiation and gravity. The models are inscribed in commercial software Fluent and Star CCM.
- Shear Stress Transport (SST) with Ross-land radiation model has given better results for Temperature, Soot and Nitrogen Oxide (NO) formation.
- Compared to two step and moss brooks in fluent, One step Soot model has given better Soot formation.
- Finally, Openfoam was used to look for chemical analysis of Methane (CH_4), and Ethylene (C_2H_4)

2 REYNOLDS-AVERAGED NAVIER-STOKES EQUATIONS AND SOOT MODEL

κ-ε Model:

In fluent $\kappa - \varepsilon$ model composed of two transport equations, which need to be solved for evaluation of Reynolds Stress, because the time average Navier-Stokes equations cannot solve the turbulence fluctuation directly, so a turbulence model is required [49].

Reynolds Stress equation is given by

$$\rho u_i^{'} u_j^{'} = \frac{2}{3}\rho\kappa\delta_{ij} + [\mu_t \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}] \tag{1}$$

Where μ_t is the eddy kinematic viscosity, δ_{ij} is Kronecker delta and κ is the kinematic energy of turbulence. $u_{i'}$ and $u_{j'}$ represent fluctuating velocity in different direction.

Two transport equation κ-ε are as follow:

$$\frac{\partial(\rho\kappa)}{\partial t} + \frac{\partial(\rho u_i \kappa)}{\partial x_i} = \frac{\partial[(\mu + \frac{\mu_t}{\sigma_k})\frac{\partial\kappa}{\partial x_i}]}{\partial x_i} + 2\mu_t E_{ij} E_{ij} - \rho\varepsilon \tag{2}$$

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial[(\mu + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial\varepsilon}{\partial x_i}]}{\partial x_i} + C_{1\varepsilon}\frac{\varepsilon}{\kappa} 2\mu_t E_{ij} E_{ij} - C_{2\varepsilon}\rho\frac{\varepsilon^2}{\kappa} \tag{3}$$

$C_{1\varepsilon}, C_{2\varepsilon}, \sigma_k, \sigma_\varepsilon$ are empirical constants and E_{ij} is the generation of turbulence. The following is the calculation of turbulent viscosity calculation.

$$\mu_t = \rho C_\mu \frac{\kappa^2}{\varepsilon} C_\mu = 0.09 \tag{4}$$

The species equation is a statement of conservation of a single species. The conservation equation for the mass fraction ($m_{i'}$) species $i^{'}$ is given by

$$\frac{\partial \rho m_{i'}}{\partial t} + \frac{\partial (\rho u_{i m_{i'}})}{\partial x_i} = -\frac{\partial}{\partial x_i} J_{i',i} + R_{i'} + S_{i'} \tag{5}$$

$J_{i',i}$ is the i^{th} component of the diffusion flux of species $i^{'}$ in the mixture, $R_{i',i}$ is the net rate of production species $i^{'}$ by chemical reaction and $S_{i'}$ is the source term from the dispersed phase or any user defined source.

κ-ω Model:

$\kappa - \omega$ turbulence model is a common two-equation turbulence model that is used as a closure for the Reynolds-Average Navier-Stokes equations (RANS). The model attempts to predicts turbulence by the turbulence kinetic energy (κ) and the specific rate of dissipation (ω) [50].

$$\frac{\partial (\rho \kappa)}{\partial t} + \frac{\partial (\rho u_j \kappa)}{\partial x_j} = \frac{\partial [(\mu + \sigma_k \frac{\rho \kappa}{\omega}) \frac{\partial \kappa}{\partial x_j}]}{\partial x_j} + P - \beta^* \rho \omega \kappa \tag{6}$$

$$P = \tau_{ij} \frac{\partial u_i}{\partial x_j} \tag{7}$$

$$\frac{\partial (\rho \omega)}{\partial t} + \frac{\partial (\rho u_j \omega)}{\partial x_j} = \frac{\partial [(\mu + \sigma_\omega \frac{\rho \kappa}{\omega}) \frac{\partial \omega}{\partial x_j}]}{\partial x_j} + \frac{\gamma \omega}{\kappa} P - \beta \rho \omega^2 + \frac{\rho \sigma_d}{\omega} \frac{\partial \kappa}{\partial x_j} \frac{\partial \omega}{\partial x_j} \tag{8}$$

Shear Stress Transport(SST) Model:

Shear Stress Transport(SST) turbulence model is widely used. It is a robust two-equation eddy-viscosity turbulence model used in Computational Fluid Dynamics. The model combines the $\kappa - \varepsilon$ and $\kappa - \omega$ turbulence model. $\kappa - \omega$ uses as inner region of the boundary layer and $\kappa - \varepsilon$ predicts for shear flow [51]. The formation of SST model is based on physical experiments and attempts to predict solutions.

$$\frac{\partial(\rho\kappa)}{\partial t}+\frac{\partial(\rho u_j\kappa)}{\partial x_j}=\frac{\partial[(\mu+\sigma_k\mu_t\frac{\rho\kappa}{\omega})\frac{\partial\kappa}{\partial x_j}]}{\partial x_j}+P-\beta^*\rho\omega\kappa \tag{9}$$

$$\frac{\partial(\rho\omega)}{\partial t}+\frac{\partial(\rho u_j\omega)}{\partial x_j}=\frac{\partial[(\mu+\sigma_\omega\mu_t)\frac{\partial\omega}{\partial x_j}]}{\partial x_j}+\frac{\gamma}{\nu}P-\beta\rho\omega^2+2(1-F_1)\frac{\rho\sigma_{\omega2}}{\omega}\frac{\partial\kappa}{\partial x_j}\frac{\partial\omega}{\partial x_j} \tag{10}$$

Soot Models:

There are two well-known turbulence models that are used for our RANS simulations. One is $k-\varepsilon$ turbulence model and the other is the Shear Stress Transport (SST) model. The $k-\varepsilon$ model solves two transport equations. k is the turbulence kinetic energy and ε is the turbulent dissipation. SST turbulence model is widely used and combines the $k-\omega$ and $k-\varepsilon$ turbulence model such that $k-\omega$ is used as the inner region of the boundary layer and $k-\varepsilon$ is used in the free stream [51].

There are three soot models in Fluent that will be used for this study. They are the one-step method (Khan and Greeves model [52], two-step method [53] and Moss-Brooks [54] method. Note that the CFD solver is Fluent. [55]

One step model:

One-step [51] model solves a single transport model for soot mass fraction:

$$\frac{\partial(\rho Y_{soot})}{\partial t}+\frac{\partial(\rho u_j Y_{soot})}{\partial x_i}=\frac{\partial}{\partial x_i}[\frac{\mu_t}{\sigma_{soot}}\frac{\partial Y_{soot}}{\partial x_i}]+R_{soot} \tag{11}$$

Where Y_{soot} is soot mass fraction, σ_{soot} is turbulent Prandlt number for soot transport, and R_{soot} is net rate of soot generation.

Two step model:

Two-step [53] Reynolds Stress Tensor soot model in Fluent predicts the generation of radical nuclei and then computes the formation of soot on these nuclei. Two-step model in

Fluent solves two scalar quantities: the soot mass fraction and the normalized radical nuclei concentration. The following equation is the two-step equation:

$$\frac{\partial(\rho b^*_{muc})}{\partial t} + \frac{\partial(\rho u_i b^*_{muc})}{\partial x_i} = \frac{\partial}{\partial x_i}[\frac{\mu_t}{\sigma_{muc}}\frac{\partial b^*_{muc}}{\partial x_i}] + R^*_{muc} \tag{12}$$

b^*_{muc} is normalized radical nuclei concentration. σ_{muc} is turbulent Prandlt number for nuclei transport and R^*_{muc} is the normalized net rate of nuclei generation.

Moss Brooks model:

The Moss-Brooks [54] model solves transport equations for normalized radial nuclei concentration b^*_{muc} and mass fraction Y_{soot}

$$\frac{\partial(\rho Y_{soot})}{\partial t} + \frac{\partial(\rho u_j Y_{soot})}{\partial x_i} = \frac{\partial}{\partial x_i}[\frac{\mu_t}{\sigma_{soot}}\frac{\partial Y_{soot}}{\partial x_i}] + \frac{dM}{dt} \tag{13}$$

$$\frac{\partial(\rho b^*_{muc})}{\partial t} + \frac{\partial(\rho u_i b^*_{muc})}{\partial x_i} = \frac{\partial}{\partial x_i}[\frac{\mu_t}{\sigma_{muc}}\frac{\partial b^*_{muc}}{\partial x_i}] + \frac{1}{N_{norm}}\frac{dN}{dt} \tag{14}$$

Where Y_{soot} is soot mass fraction, M is soot mass concentration (kg/m^3). b^*_{muc} is the normalized radical nuclei concentration and N is soot particle number density ($particles/m^3$)

Radiation modeling

Heat transfer interacts with other physics when optimizing and verifying system and product designs. Radiation is one of them. Conduction, radiation, inter diffusion heat transfer occurs in the combustion system.

Combustion is speedy oxidation generation of heat and radiation. Combustion is so important because of the intrinsic importance of chemical reaction. Thermal radiation is an important energy transport process at high temperature that needs to be considered for implementation of practical combustion system. Radiation does not directly affect the reaction processes, but the transfer of radiation indirectly affects the flame temperature distribution and chemical reactions. In 2005 Chan and Viskanta showed that Radiation can significantly affect the flame temperature, minor species, the NOx emissions, soot formation, flame extinction, and other phenomena.

P-1 model

In P1 model reflection of incident radiation at the surface is isotropic. There is a loss of accuracy depending on the complex geometry. P1 model over predict radiate fluxes from heat sources or sinks. [55]

$$\nabla.(\Gamma\nabla)G - aG + 4a\sigma T^4 = S_G \tag{15}$$

Where σ is the Stefan-Boltzmann constant and S_G is a user-defined radiation source. Fluent solves this equation to determine the local radiation intensity when the P-1 model is active. [55]

Rosseland model

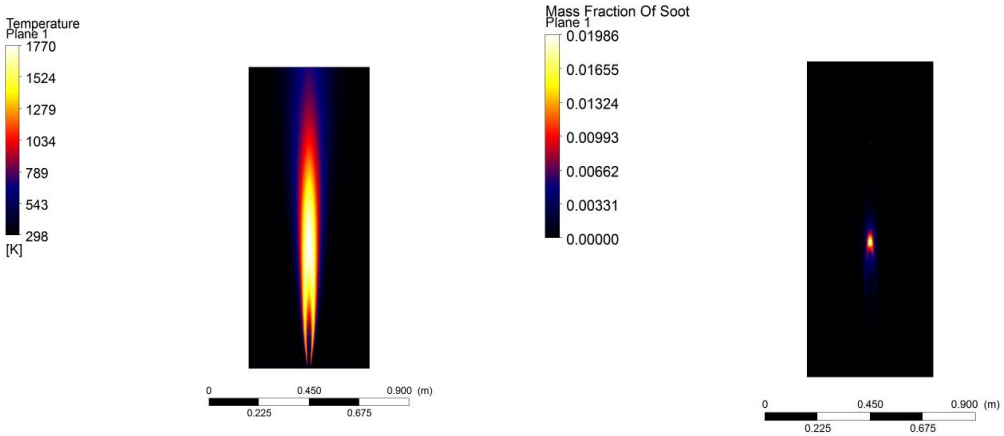
Rosseland model does not solve an extra transport equation, so it is faster than P1 model and requires less memory. Rosseland model is only for optically thick media and available only with segregated solver. [55]

$$q_r = -16\sigma\Gamma n^2 T^3 \nabla T \tag{16}$$

$$q = q_c + q_r = -(k + k_T)\nabla T k_T = 16\sigma\Gamma n^2 T^3 \tag{17}$$

Where k is the thermal conductivity and k_T is the radiative conductivity.

Results:



7 (a) 7 (b)

Figure 7: 7 (a) contour plot of temperature of the ethylene flame and 7 (b) contour plot of mass fraction of soot.

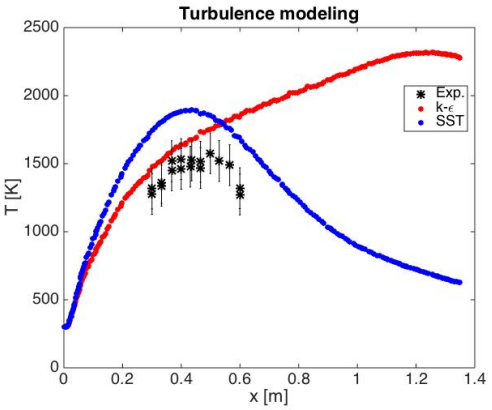
The experiment from Coppalle and Joyeux [1] is the flame that we will compare our simulations too. The flame is an ethylene diffusion flame at a Reynolds number of 5700. The inlet velocity is 6.3 m/s (ethylene) and the diameter (D) of the jet is 9 mm. The computational domain is 150 D long and radius of the domain is 30 D.

Figure 1 (a) shows the flame and the computational domain of the flame. Figure 1 (b) is a contour plot of soot. Note that we did not tune any coefficients in the models that were used (turbulence, soot and radiation). Also, all plots below that compare to experimental data are at the centerline of the axis.

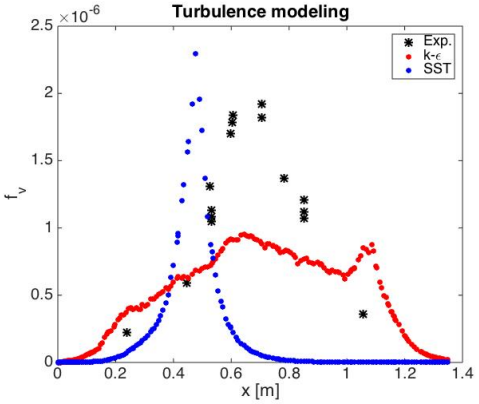
Figure 2 illustrates the importance and effect of turbulence modeling on temperature and soot generation. The error bars in Figure 2 (a) include the rms of temperature and it shows temperature fluctuation about the mean. Note that gravity is "on" for Figure 2. After comparing with experimental results Coppalle and Joyeux [1] from Figure 2 (a) and 2 (b) with no radiation, SST model has better results for temperature and soot formation. Turbulence models are $k - \epsilon$ and SST.

Additionally, when gravity is turned "on" or "off" in Figure 3 and Figure 4, temperature and soot generation also varies. When gravity is turned "off", the flame crosses the boundary as shown in Figure 4 (b). Figure 3 and 4 illustrates the effect of gravity on the flame and that it should be included. Figure 5 (a) is a plot of temperature showing the effect of different soot models on temperature and Figure 5 (b) is a plot of soot with the different soot models. Figure 5 (b) depicts that one step soot model has better results compared to the other two models (two-step and Moss-Brooks)

When radiation is turned "off" for SST with gravity for one step soot model, NO_X formation is higher than radiation "on". When radiation is considered, temperature is not enough for the formation of necessary concentration of atomic oxygen by heat dissociation. It can be stated for reduction of NO_X emission. Lower temperature thin film is much more effective compared to higher temperature combustion as shown in Figure 6 (b) and 7 (a). Figure 6 illustrates with SST turbulence modeling, Rossland radiation and with one step soot modeling shows that effect on NO_X formation.

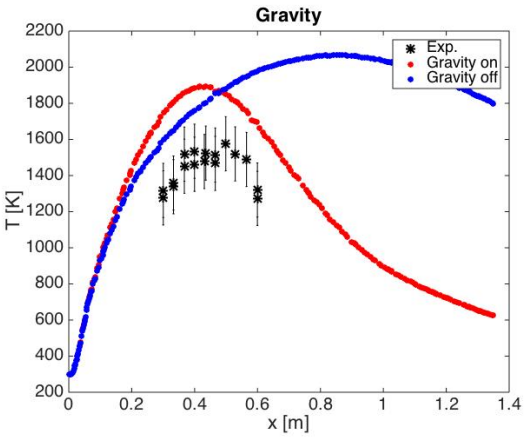


8 (a)

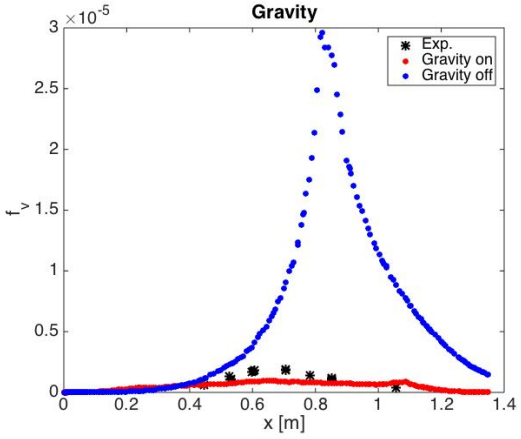


8 (b)

Figure 8: 8 (a) is a plot of temperature with different turbulence models and 8 (b) is a plot of soot volume fraction with different turbulence models with no radiation.

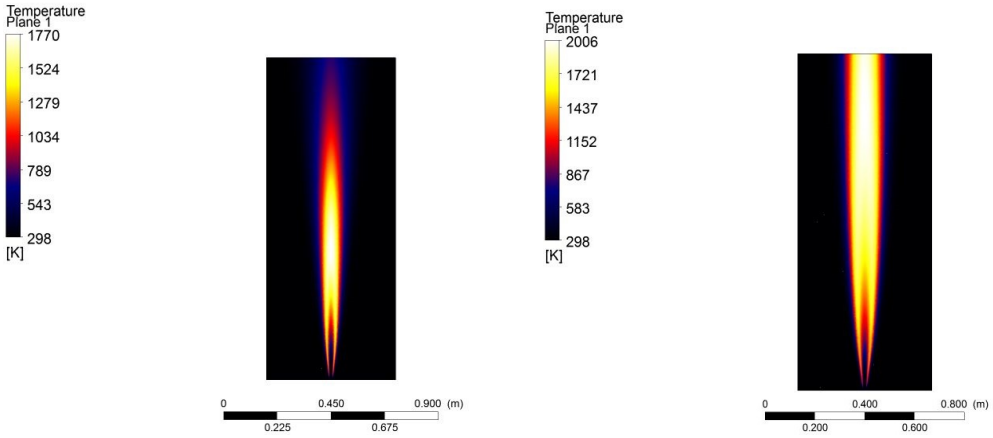


9 (a)



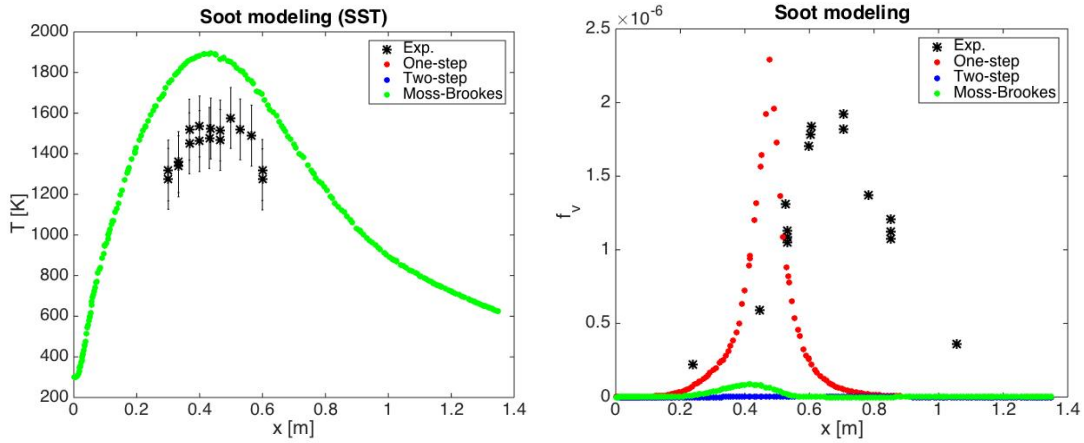
9 (b)

Figure 9: 9(a) Effect of gravity on SST with no radiation for Temperature and 9(b)Effect of gravity on SST with no radiation for Soot.



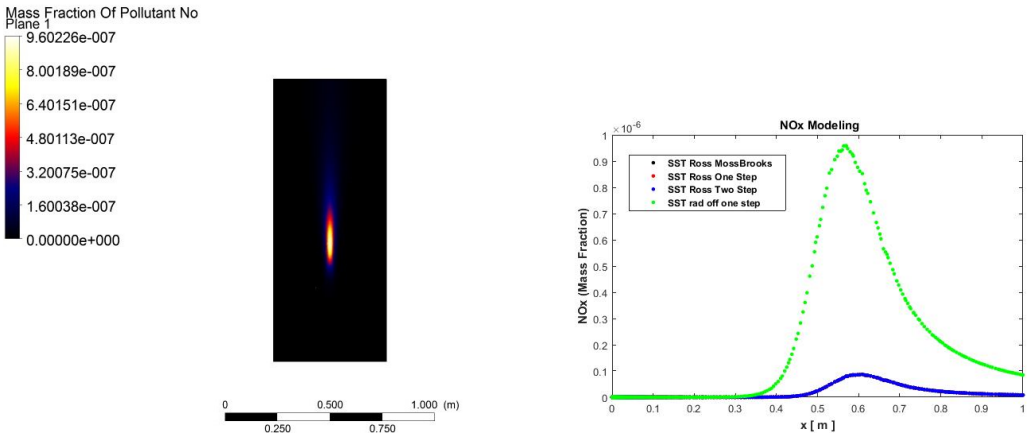
10 (a) 10 (b)

Figure 10: 10 (a) is a contour plot of temperature propagation when gravity is tuned "on" and 10 (b) is a contour plot of temperature propagation when gravity is tuned "off".



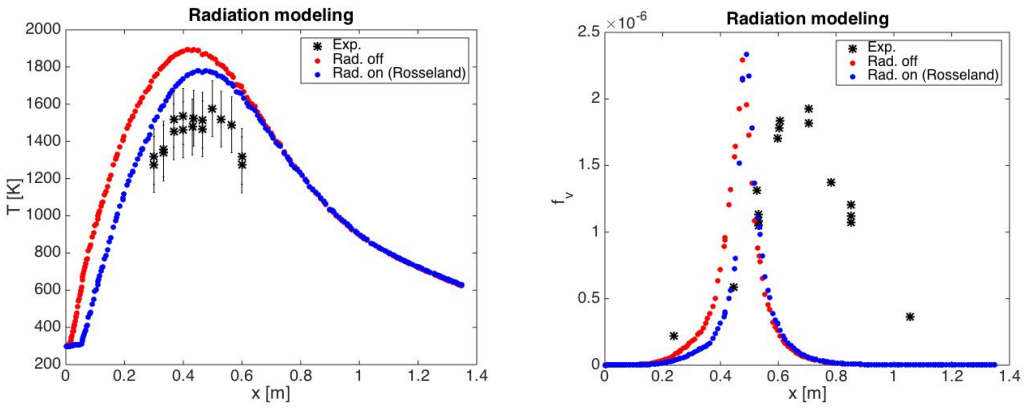
11 (a) 11 (b)

Figure 11: 11 (a) is a plot of temperature showing the effect of different soot models and 11 (b) is a plot of soot with different soot models of SST with no radiation.



12 (a) 12 (b)

Figure 12: 12 (a) is a contour plot of NOx formation without gravity and 12 (b) is plot of NOx modeling.

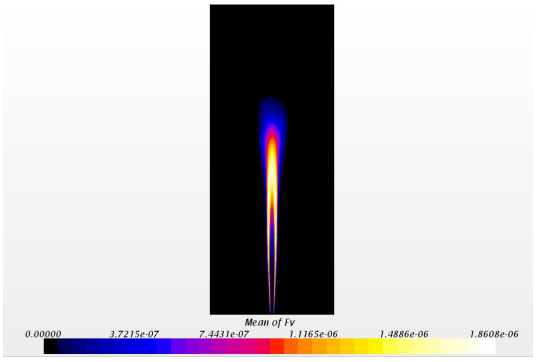


13 (a) 13 (b)

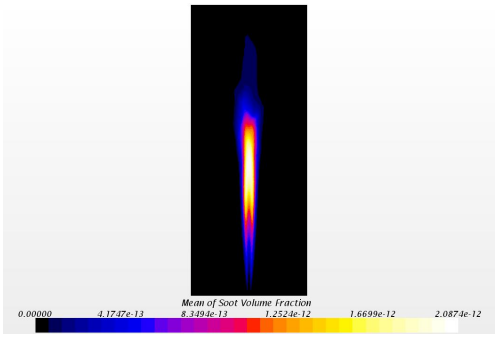
Figure 13: 13 (a) Rosseland radiation modeling for Temperature 13 (b) Rosseland radiation modeling for Soot.

Flamelet Radiation model:

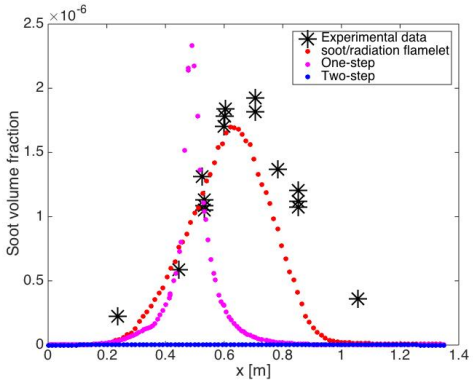
Literature from Modest et al. [7] and Wang et al. [56] states that a strong coupling between temperature and soot. Therefore, a flamelet radiation model with optical thick radiation was developed to include radiation with a flamelet library. The inclusion of the two-equation soot flamelet model from Carbonell et al. [2] is used. Details of the model and equations are given in Doom [3]. Figure 8 shows results that include soot and radiation flamelet modeling. Figure 8 (a) is a contour of soot volume fraction of the soot and radiation flamelet model and Figure 8 (b) is a contour of soot volume fraction of the soot model used in a commercial code. Figure 8 (c) is a centerline plot of soot volume fraction of the experimental data Coppalle and Joyeux [1], soot/radiation flamelet model and soot models from commercial software. The commercial code soot models are the one-step and two-step model.



14 (a)



14 (b)



14 (c)

Figure 14: This figure illustrates the difference between flamelet soot radiation model and the soot modeling implemented in a CFD solver.

OpenFOAM:

Computational Fluid Dynamics (CFD) development is the move away from experimental studies and it is more empirical and accurate applicable mathematics in engineering. It works on both Windows and Linux platform. There is no needed any License for solving the computational fluid dynamics problems. Open-source codes are available at www.openfoam.com. [57] This code is written in C++ that reasonably makes straightforward to implement new models and fit them into the whole code structure. Additionally, OpenFOAM is being continuously developed. Here recent version of OpenFOAM (v1712) is used. Here, reacting diffusion flame is simulated for Methane and Ethylene and contour plots are compared each other. Moreover, full reaction mechanism is incorporated and investigated in the formation of Hydroxide (OH), Hydrogen peroxide (H_2O_2), Nitrogen Oxide (NO) and water (H_2O) for Methane (CH_4) and Ethylene(C_2H_4).

Fluent mesh can be incorporated in OpenFoam by using fluentMeshToFoam command. New FOAM mesh is saved in constant/polyMesh folder. In the new mesh inlet, outlet, air, wall name has been renamed with 0 directory folder. If it does not match, the simulation will not work. Here block mesh is used for meshing. Here, it is a laminar flow reacting diffusion flame simulation. For methane(CH_4) the reacting chemistry was set up as follow and Nitrogen (N_2) gas is inert :

$$CH_4 + 2O_2 = CO_2 + 2H_2O \tag{18}$$

For Ethylene reacting equilibrium as follow:

$$C_2H_4 + 3O_2 + 11.28N_2 = 2CO_2 + 2H_2O + 11.28N_2 \tag{19}$$

After being set up these basic parameter we can set the initial temperature and outlet temperature. Here temperature is not tuned and kept as 293 K for initial air and fuel

temperature and 2000 K as the outlet temperature. Also the wall temperature is kept as 293 K and for fuel and air velocity were 1 m/s respectively. After setting up the parameters the solver is defined for running the simulation. Here the starting and ending time were 0 and 0.5 respectively. Also the time difference delta was 1e-6. Additionally, for faster simulation the simulation is setup in cluster and 4 processors are used. Processors can be increased to 8 or 16.

The main reason for combustion simulation on OpenFOAM was to figure out the species of combustion products. Hydroxide(OH), Hydrogen per-oxide(H_2O_2) are the main reason for soot formation. Figure 12 shows the reaction between Benzine (C_6H_6) and Hydroxide (OH) for soot formation. Firstly OH is oxidized then it is agglomerated. After that precursor molecules are grown by surface reaction and coagulation. Particle inception occurs and molecular weight is grown. Molecules are then reacted with Benzine(C_6H_6) and Poly- cyclic Aromatic Hydrocarbon (PAH) is formed. If Hydroxide (OH) and Hydrogen Per-oxide (H_2O_2) becomes higher, the soot formation will be higher [58]. Diffusion combustion simulation for methane was default set up. After Methane combustion simulation Temperature, Hydroxide (OH), Water (H_2O), Hydrogen Per-Oxide (H_2O_2), Nitrogen Oxide (NO) formation were found. After that fuel was changed to Ethylene (C_2H_4) and contour plots are compared with Methane (CH_4) for looking, how the Ethylene (C_2H_4) combustion products formation varied. For graphical representation we needed GNU plot. In order to GNU plot python was used. Here graphical plots are not shown. Figure 13 shows the two fuel (CH_4 and C_2H_4) comparison. Diffusion flame for Methane (CH_4) was done first. For different fuel the combustion products formation will be different. However, the changing fuel shows that the set up is appropriate. Figure 14 (a) and 14 (b) are Temperature contour plot for Methane and Ethylene respectively. Highest temperature for Methane and Ethylene combustion were 1873 K and 1681 K respectively. For Methane and Ethylene highest Hydroxide (OH) formation were 1.895e-03 and 6.656e-04 subsequently are shown in figure 15. Figure 16 is contour plot of water (H2O)

here for methane highest water formation is 3.525e-02 and for ethylene it is 2.341e-02. Figure 17 is a contour plot for hydrogen peroxide (H2O2) formation. For methane highest H2O2 formation is 1.2e-06 and for ethylene it is 3.201e-07. Highest level of Nitrogen Oxide (NO) formation for methane was 9.427e-05 and for ethylene the NO formation was lower and it is 1.083e-04 as shown in figure 18.

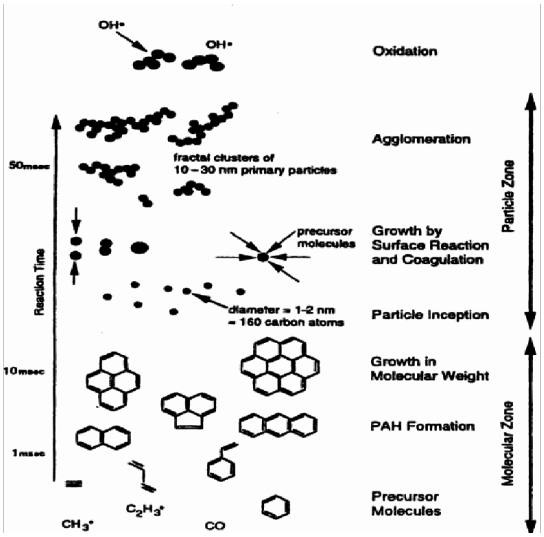
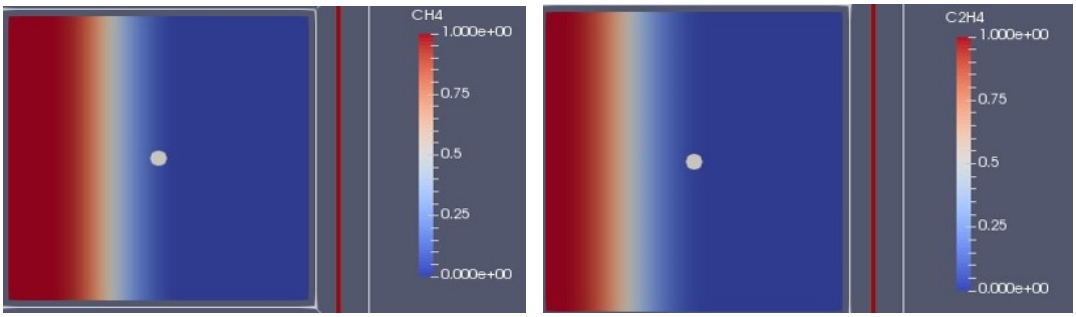
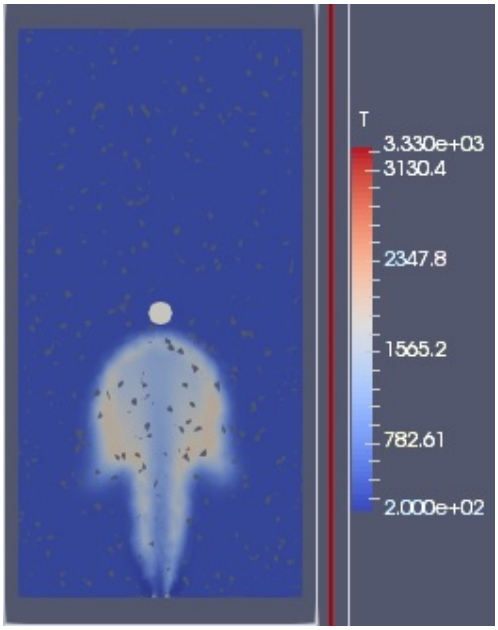


Figure 15: Chemistry of Soot formation [Bockhorn 1994].

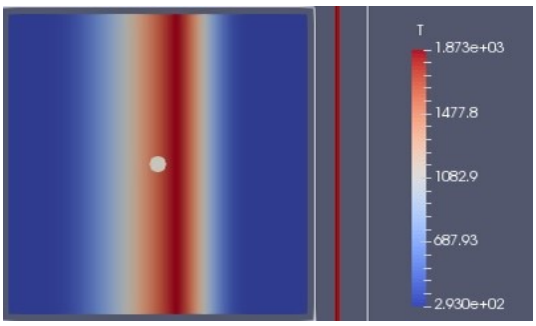


16 (a) 16 (b)

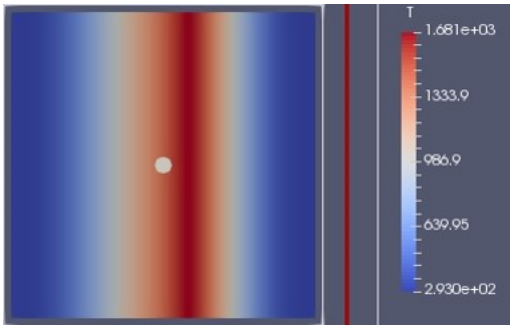
Figure 16: 16 (a) is a contour plot of Methane (CH_4) showing the CH4 fuel and 16 (b) is a contour plot of Ethylene (C_2H_4) showing the C_2H_4 fuel.



17 (a)

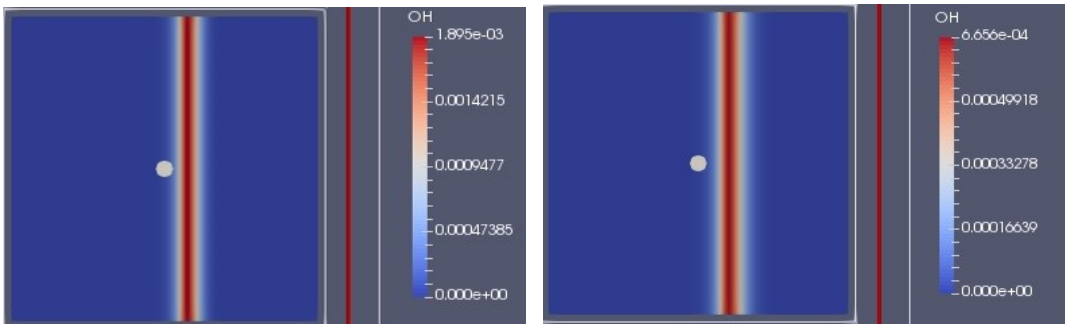


17 (b)



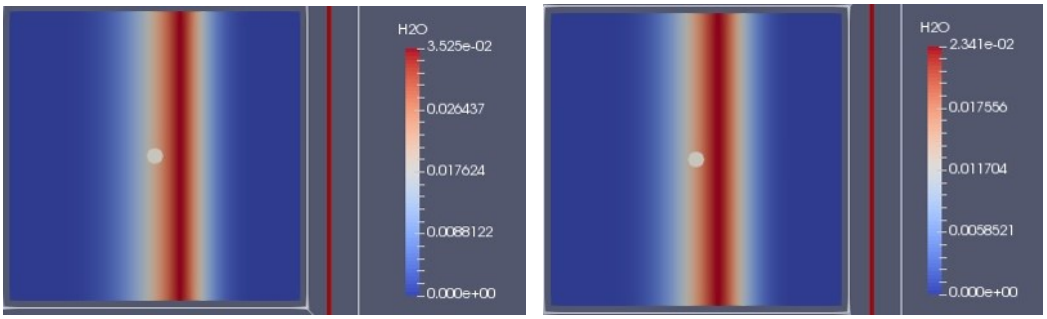
17 (c)

Figure 17: 17 (a) Combustion flame 17 (b) is a contour plot of Methane (CH_4) showing the Temperature formation and 17 (c) is a contour plot of Ethylene (C_2H_4) showing the the Temperature formation.



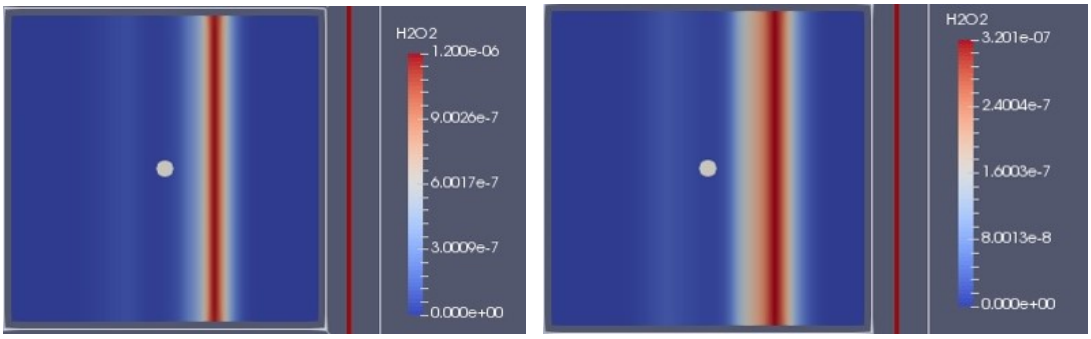
18 (a) 18 (b)

Figure 18: 18 (a) is a contour plot of Methane (CH_4) showing the Hydroxide (OH) formation and 18 (b) is a contour plot of Ethylene (C_2H_4) showing the Hydroxide (OH) formation.



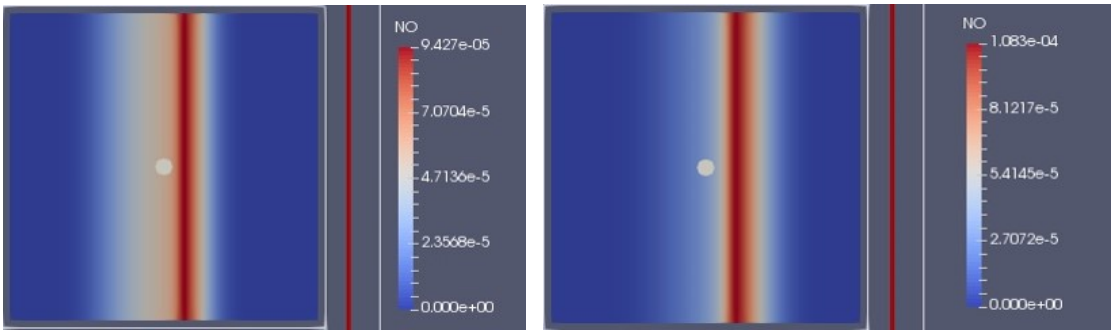
19 (a) 19 (b)

Figure 19: 19 (a) is a contour plot of Methane (CH_4) showing the Water (H_2O) formation and 19 (b) is a contour plot of Ethylene (C_2H_4) showing the Water (H_2O) formation.



20 (a) 20 (b)

Figure 20: 20 (a) is a contour plot of Methane (CH_4) showing the Hydrogen Per-Oxide (H_2O_2) formation and 20 (b) is a contour plot of Ethylene (C_2H_4) showing the Hydrogen Per-Oxide (H_2O_2) formation.



21 (a) 21 (b)

Figure 21: 21 (a) is a contour plot of Methane (CH_4) showing the Nitrogen-Oxide (NO) formation and 21 (b) is a contour plot of Ethylene (C_2H_4) showing the Nitrogen-Oxide (NO) formation.

Future Work

OpenFOAM can be used to implement modified equation. Here in combustion simulation problem the vortex ring can be implement for laminar flow. Additionally, the simulation can be done for different fuel and the chemical analysis can be investigated. In future combustion with obstacle simulation can be solved. Mainly gaseous reaction will be investigated. I have an intention to look at the chemical analysis during the Large Eddy Simulation (LES). OpenFOAM can do the Direct Numerical Simulation (DNS). In future I may look at some modified combustion ring for Direct Numerical Simulation (DNS). Synergies gas combustion can also be investigated. Finally, modified Naiver-Stokes equation will be implemented for looking the combustion products such as Carbon mono-oxide(CO), Soot, Nitrogen Oxide (NO). The Radiation model will also be included for this combustion simulation such as P1, Ross-land radiation model. The radiation model will be also be modified to find out some new model that can give better results.

3 CONCLUSION

CFD is used to study soot formation in an ethylene air diffusion flame. The inclusion of the SST turbulence model, gravity, one-step soot model and Rossland radiation provide good agreement with experimental data of an ethylene diffusion flame using commercial software. The study also indicates that when other RANS models are used, soot formation varies, but not reasonable compared to SST turbulence model, gravity, one-step soot model. Rossland radiation model has also great effect on NO_X formation. Finally, the inclusion of the two-equation soot flamelet model from Carbonell et al. [2] and the flamelet radiation model from Doom [3] agreed with experimental data as well. Diffusion combustion simulation for Methane (CH4) and Ethylene (C2H4) were compared each other for verifying set up and simulation. The Ethylene diffusion simulation was matched with Methane and the results are reasonable.

APPENDIX

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