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Comparative Study with Numerical Simulation of Fossil Fuels Combustion for Industrial Furnaces

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Abstract: *The selection of liquid or gas fuel to be used in an industrial furnace can be of extreme importance, having a direct effect on its performance, of the equipment. These factors are highly dependent on the combustion process and on factors such as the flame shape droplet path, temperature variation and heat flux distributions within the furnace. In the present work, numerical simulations were carried out, using the finite volume method, with the purpose of analyzing and comparing the combustion process inside a furnace when operating with three types of fuel: Pentane, Hexane and Heptane all are reacting with air with different mass flow rate and air velocity. The results will be showing the temperature distribution, droplet profiles, and mass fraction of emissions. Liquid fuels or high hydrocarbon have a great advantages over other low carbon fuels because they are in liquid form so that they are easily vaporized in combustion process and there is no need for compressing the fuels. Simulation results shows that Heptane fuel has released great amount of energy and high temperature profile as compare to other liquid fuels. Emission after the combustion process is lowest in high hydrocarbon fuel because of rapid evaporation and high combustible in nature.*

Key words: Hydrocarbons, Fossil fuels, Furnaces, CFD, Emissions, Combustion, Liquid fuels, Fluent 14.5.

I. INTRODUCTION

A. Furnace

A furnace is essentially a thermal enclosure and is employed to process raw materials at high temperatures both in solid state and liquid state. Several industries like iron and steel making, non ferrous metals production, glass making, manufacturing, ceramic processing, calcinations in cement production etc. employ furnace. The principle objectives are

- 1) To utilize heat efficiently so that losses are minimum,
- 2) To handle the different phases (solid, liquid or gaseous) moving at different velocities for different times and temperatures such that erosion and corrosion of the refractory are minimum.

B. Source of energy

- 1) Combustion of fossil fuels, that is solid, liquid and gaseous.
- 2) Electric energy: Resistance heating, induction heating or arc heating.
- 3) Chemical energy: Exothermic reactions

C. Types of furnaces

Furnaces are both batch and continuous type. In the continuous type for example in heating of ferrous Material for hot working, the furnace chamber consists of preheating, heating and soaking zones. The material enters through the preheating zone and exits the soaking zone for rolling. But the flow of products of combustion is in the reverse direction. Furnace design is recuperative type in that material exits at the desired temperature from the soaking zone and the products of combustion discharge the preheating zone at the lowest possible temperature. Different types of continuous furnaces are in use, like walking beam type, pusher type, roller hearth type, screw conveyor type etc. In the batch furnaces, the load is heated for the fixed time and then discharged from the furnace. There are different types of batch furnaces like box type, integral quench type, pit type and car. In many cases the furnace is equipped with either external heat recovery system or internal heat recovery system. In the external heat recovery system a heat exchanger like recuperator is installed outside the furnace. Here heat exchanger must be integrated with the furnace operation. In the internal heat recovery the products of combustion are recirculated in the furnace itself so that flame temperature is somewhat lowered. The objective is to reduce the NO_x formation Ottom type

All fossil fuel contain potential energy. On combustion potential energy is released in the products of combustion. The products of combustion exchange energy with the sink to raise its temperature to the required value and then exit the system. The sensible heat in POC (products of combustion) at the critical process temperature is not available to the furnace. The higher the process critical temperature higher would be the sensible heat in POC. This sensible heat in POC is very important from the point of view of fuel utilization. We define gross available heat (GAH) as $GAH = \text{Calorific value of fuel} + \text{sensible heat of reactants} - \text{Heat carried by POC}$

GAH represents the heat available at the critical process temperature; it may not represent heat available to perform a given function due to the various types of losses. GAH may be used as a criterion for comparing different fuel-combustion system. Once the furnace is designed and built, the heat losses are not within the control of the operator; it is governed by the process critical temperature, refractory lining thickness and thermal conductivity of the refractory. Defining net available heat (NAH) as $NAH = GAH - \text{Heat losses}$. NAH can be used as a criterion for comparing the smelting/melting/heating efficiency of different furnaces.

1) **Heat Utilization:** Concepts Efficient utilization of fossil fuel reserves requires, in addition to other factors, utilization of heat of POC exiting the furnace. It is well known that potential energy of fuel at 25° C on combustion is converted into the sensible heat pf products of combustion at the flame temperature. Products of combustion after transferring their heat to the furnace chamber exit the furnace. Heat carried by products of combustion depends on the temperature of the furnace; higher is the furnace temperature higher is the amount of heat carried by POC. It may range somewhere in between 40 to 60% of the calorific value of fuel. Heat of POC can be recovered either external to the furnace by installing a heat exchanger or internally by recirculating the POC into the flame in the furnace itself. The former is called external heat recovery and the later is internal heat recovery. In the following we discuss the principles of external heat recovery of POC. Normally a heat exchanger is integrated with the furnace which captures and reuses the heat of POC simultaneously.

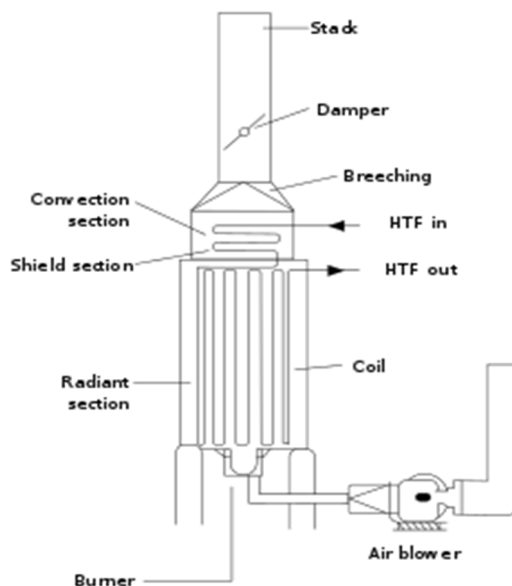


Figure: 1 Schematic diagram of an industrial process furnace

Numerical modelling is an important device inside the design and optimization of commercial combustion equipments. Programs encompass the optimization of the combustion process, for more strength efficient Operations and the discount of green residential gases (GHGs) emissions, as well as the prediction of pollutants emissions along with CO(carbon monoxide), SO_x (sulfur oxides), and NO_x (nitrogen oxides).Pollution prediction in combustion systems is turning into an increasing number of crucial due to multiply necessity of environmental policies enforcement. For instance, the formation of nitrogen oxides (NO_x) in air-feed combustion structures represents a significant source for this pollutant inside the industrial quarter. Because of the arena-huge boom in the use of fossil fuels, pollutant emissions control has turned out to be a trouble of global difficulty. Moreover, with increasing oil costs, the use of lower quality fuels will have a tendency to exacerbate the hassle. Advances in computational modelling have

resulted in an extensive utility of numerical simulations in industrial furnaces, imparting insights and improving the information of the combustion operation. Distinctive analyses of the effects of the combustion method when the use of special fuels and oxidants, as well as one of a kind situations, offers the method for achieving a cleaner and extra efficient operation.

Computational fluid dynamics (CFD) modelling is now widely implemented as a commercial plant improvement and technique optimization device. The constant boom in computer strength over the latest years has enabled manner engineers to model reacting multi-phase flows in practical geometry with excellent mesh resolution. As an end result, the number of applications of CFD to industrial tactics is likewise growing rapidly and growing in sophistication. This paper reviews a number of the latest packages of the CFX-four code [CFX-4.3: Solver Manual, AEA Technology Engineering Software, 1999] of the electric era and combustion industries. The aim is to show what may be performed and also to identify developments and those regions in which further paintings are needed. Examples make up of coal-fired low NO_x burner layout, furnace optimization, over-fireplace air, gas re-burn, and laminar flames. It is argued that the fashion is for CFD models to grow to be more comprehensive and reachable by way of being coupled to different technique models and embedded in computerized facts and system management structures.

II. LITERATURE

R. Novella 1 Spray ignition and flame stabilization in the frame of diesel-like combustion conditions combine fundamental and complex physical and chemical processes. In this work, a numerical investigation has been performed to evaluate the potential of integrating detailed chemistry into CFD calculations, in order to improve predictions and gain more insight in involved processes. This work has been carried out using the capabilities of Open FOAM ©code, which provides an open source framework for 3D-CFD simulations ,including an ODE solver for solving chemical kinetics. As a general methodology, this study is based on simulating free n-heptane sprays injected into a constant volume vessel, corresponding to the conditions of the experimental database provided by Sandia National Laboratories. Calculations results have been compared to experiments, evaluating the effect of a wide range of ambient conditions on spray ignition and combustion characteristics. Specifically, this research checks the performance of some relevant n heptanes oxidation mechanisms found in the literature, with different degree of complexity , for modeling the chemical history of the fuel. The results of this investigation show there lative influence of chemical mechanism on spray/flame structure in terms of ignition delay and also ignition and flame stabilization sites. The comprehensive mechanism performs generally better than more simplified chemistry models. However, its accuracy is also compromised for modeling advanced diesel-like combustion concepts based on injecting the spray into a low oxygen concentration environment. **Amin Maghbouli 2**Dual-fuel combustion provides a relatively easy and inexpensive alternative to conventional diesel engine combustion by drastically reducing fuel consumption with comparable performance characteristics. Accurate simulation of the dual-fuel combustion requires utilization of a detailed chemistry combined with a flow simulation code. In the present study, the combustion process within the diesel and diesel/gas dual-fuel engine is investigated by use of a coupled 3D-CFD/chemical kinetics framework. In this study, methane and n-heptane are used as representatives of the natural gas and diesel fuels. The multi-dimensional KIVA-3V code, with modified combustion and heat transfer models, incorporates a chemical kinetics mechanism for n-heptane and methane oxidation chemistry. The source terms in energy and species conservation equations due to chemical reactions are calculated by integrating the CHEMKIN chemistry solver into the KIVA code. The model is applied to simulation of a medium duty dual-fuel converted diesel engine. A chemical kinetics mechanism which consists of 42 species and 57 reactions is used for prediction of n-heptane oxidation chemistry. Simulation of dual-fuel combustion is performed using the same mechanism with addition of a series of major methane oxidation pathways. The results show that Zheng and Yao's n-heptane mechanism which had been previously validated in their work, can model the diesel and dual-fuel combustion, where fuel-rich zones are present. The predictive model of this study is validated using available published experimental data. Results show that pressure and ignition delay predictions are in good agreement with experiments. Based on constant total mixture input energy in dual-fuel combustion, increasing pilot fuel amount leads to shorter ignition delay and peak pressure increment. It is found that concentrations of NO_x and CO emissions tend to increase athigher pilot fuel injection quantities. **Viswanath R. Katta 3** Computational fluid dynamics (CFD)-based predictions are presented for non premixed and partially premixed flames burning vaporized n-heptane fuel. Three state-of-the-art chemical kinetics models are incorporated into a time-dependent, two-dimensional, CFD model known as UNICORN. The first mechanism is the San Diego (SD) mechanism (52 species and 544 reactions), the second one is the Lawrence Livermore National Laboratory (LLNL) mechanism (160 species and 1540 reactions), and the third one is the National Institute of Standards

and Technology (NIST) mechanism (197 species and 2926 reactions). Soot model based on acetylene, and radiation model based on optically thin media assumption are included. Two dimensional calculations are made for the detailed structures of non premixed and partially premixed flames, strain-induced extinction and diffusion-controlled auto ignition and the results are compared with the available experimental data. Diffusion-controlled auto ignition characteristics are also compared with the ignition delay times calculated in homogeneous stoichiometric mixture of n-heptane and air. Through the simulation of complete flow fields between the opposing fuel and air ducts reasons for the flame curvature seen in some experiments are explained. Compared to the traditional one-dimensional models for opposing-jet flames, two-dimensional simulations are found to give results closer to the experimental values when the flames are highly stretched. While LLNL mechanism predicted extinction of a non premixed flame better, NIST mechanism predicted the auto ignition behavior in the flow field established by the opposing jets of fuel and heated air better. However, all three mechanisms predicted both the non premixed and partially premixed n-heptane flames very well. Surprisingly, SD mechanism with less than one-third of the species used in the other two mechanisms predicted flame structures with nearly the same accuracy. Comparisons made with the available experimental data could not suggest which mechanism is better in predicting the minor species concentrations. Computations also could not predict the temperature rise detected in the experiments in the premixed-combustion zone of a partially premixed flame when it was subjected to a moderately high stretch rate. Ravi Inder Singh 4
The increase in application

III. OBJECTIVE OF THE STUDY

Our main aim of this study to compare the different type liquid hydrocarbons like Pentane , Hexane and Heptanes . Liquid hydrocarbons have greater advantages on the other solid hydrocarbons because they are easily vaporized and highly combustible in nature due to this extra process of compressing the fuels is not needed in combustion. This dissertation with the aim to make some relation between the mass flow rate of the fuel and the air velocity in the burner. We are going to study the effect of mass flow rate, velocity of the air supplied and combustion of liquid fuels (Pentane, Hexane and Heptane).With this study we can select the suitable fuel for industrial furnaces according to combustion rate and emissions. Naphthas are a general name given to the C5 - C7 hydrocarbons. These may be found in a variety of solvents for paint, paint thinners, and Bar-B-Q lighter fluids. These are easily vaporized and highly combustible.

IV. PROBLEM FORMULATION

As the literature we have know the demand in the industry of combustion of liquid fuel. we have considered the liquid fuel combustion system. A liquid spray of PENTANE, HEXANE and HEPTANE fuel enters in a 2D duct in which air is flowing at 650 K and 1.0 m/s. The duct walls are held at a constant temperature of 1200 K. The model includes a duct length of 10 H where H is the duct height (1.0m). The Reynolds number based on inlet conditions is roughly 100,000 and the flow is turbulent. As fuels evaporate, it enters the gas phase and reacts. The combustion is modeled using the mixture-fraction/probability density function approach, with the equilibrium mixture of chemical species. The spray is assumed to consist of 100 micron diameter liquid droplets injected at 300 K over a filled spray half-angle of 30 degrees at the duct centerline. Different mass flow rate of liquid fuel is taken (0.004kg/s, 0.002kg/s, 0.006kg/s) corresponding to very fuel-lean conditions in the flow. It gives the comparisons of the combustion process and projection of fuel flows come out from the burner, temperature of flame, mass fraction, vaporization rate, droplet trajectories, mean mixture fraction etc

A. Problem-Solving With Cfd

There ar many selections to be created before putting in the matter within the CFD code. a number of the selections to be created will include: whether or not the matter ought to be second or 3D, which kind of boundary conditions to use, whether or not or to not calculate pressure/temperature variations supported the air flow density, that turbulence model to use, etc. The assumptions created ought to be reduced to grade as easy as doable, however still retentive the foremost vital options of the matter to be solved so as to achieve AN correct answer.

After the higher than selections are created, the pure mathematics and mesh is created. The grid ought to be created as fine pro re nata to create the simulation 'grid independent'. to work out the fineness needed, a grid dependence study is often dispensed by creating a series of refinements on AN ab initio course grid, and polishing off simulations on every to work out once the key results of interest don't amendment, at that purpose the grid is taken into account freelance. during this project, a grid with close to fifty,000 cells was chosen when polishing off such a study. to achieve a converged answer, relaxation factors and acceleration devices is

chosen. during this project, relaxation factors for all the parameters to be solved and therefore the GAMG smooth-solver for pressure were accustomed assist in convergence and speed optimization.

Finally, to make sure accuracy of the simulations, they must be valid against experimental knowledge. This project's simulation results are compared to AN experimental study reported within the literature .Details of the warmth money handler pure mathematics, initial boundary conditions associated with flow and temperature were followed as closely as doable once building this CFD model.

V. METHODOLOGY

Pre-processing

A. CAD Modelling:

Creation of CAD Model by exploitation CAD modelling tools for making the pure mathematics of the part/assembly of that we wish to perform FEA.CAD model could also be second or 3d.

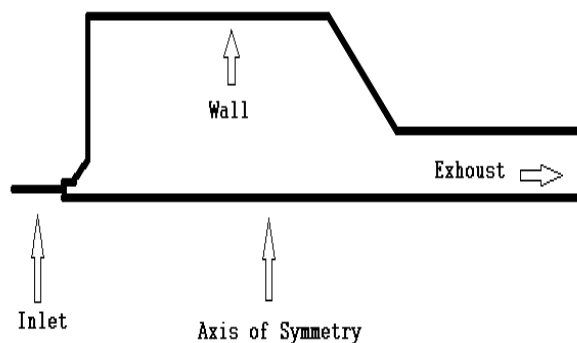


Figure -2 CAD Model of the Propeller

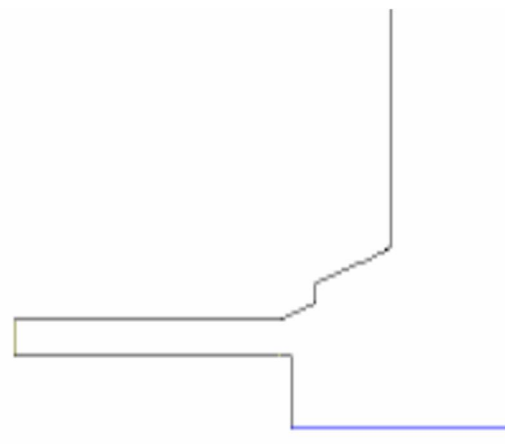


Figure - 3 Close up of the Burner

B. Meshing

Meshing may be a essential operation in CFD. During this operation, the CAD pure mathematics is discretized into massive numbers of little component and nodes. The arrangement of nodes and component in house in a very correct manner is named mesh. The analysis accuracy and period depends on the mesh size and orientations. With the rise in mesh size (increasing no. of element), the CFD analysis speed decrease however the accuracy increase.

Type of Solver: select the problem solver convergent thinker for the matter from Pressure primarily and density based solver. Physical model: select the desired physical model for the matter i.e. laminar, turbulent, energy, multiphase, etc. Material Property: select the fabric property of flowing fluid. Boundary Condition: outline the specified condition for the matter i.e. velocity, mass rate of flow, temperature, heat flux etc.

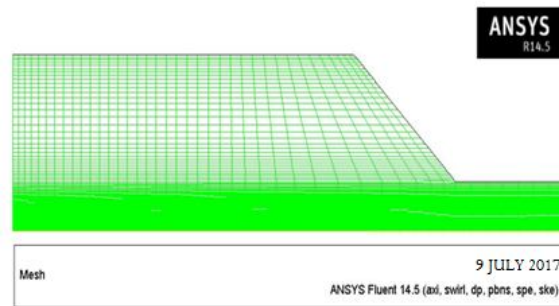


Figure -4 Mesh Model

C. method for pentane, hexane and heptane (liquid fuels)

- 1) Pressure based
- 2) Axis symmetric swirl in the 2D space list.
- 3) Gravity is enable enter -5.91 for X under gravitational acceleration

D. Model for pentane

- 1) Energy equation is enabled
- 2) K-epsilon turbulence model is used.
- 3) P-1 radiation model is used since it is quicker to run .However they DO radiation model can be used for more accurate result in typical models.
- 4) Finite rate/Eddy dissipation in turbulence chemistry interaction is used for species model.

E. Material- pentane

- 1) Mixing law is used
- 2) Thermal conductivity: - Define two polynomial coefficients
(a) 0.0076736 (b) 5.8837×10^{-5}
- 3) Polynomial coefficient for viscosity
(a) 7.6181×10^{-6} (b) 3.2623×10^{-8}
- 4) For absorption coefficient take wsggm domain.
- 5) Scattering coefficient is 1×10^{-9}
- 6) Define molecular weight is 16.313 and -10629e+8 standard state enthalpy for fuel under material type mixture.

F. Boundary conditions:

- 1) *Velocity inlet* :- select velocity profile U for axial velocity and velocity profile W for swirl velocity turbulence intensity is 17% and turbulence length scale is 0.007 Condition of velocity inlet
 - a) Temperature 312K
 - b) Mass fraction for O_2 is 0.2315
- 2) *Velocity inlet*
 - a) Radial velocity is 157.25 m/sec
 - b) Turbulence intensity 5 %
 - c) Turbulence length scale is 0.0009
 - d) Temperature 308 k
 - e) Species: - mass fraction for fuel is 0.97 and for CO_2 is 0.008.
- 3) *Out flow* :-
 - a) 5% is back flow turbulent intensity

- b) 0.6 m back flow hydraulic diameter
c) Temperature is 1300 k mass fraction for O_2 is 0.2315

G. Condition for Pressure Outlet:

Wall Name	Zone	Temperature (K)	Internal Emissivity
Wall-6		1370	0.5
Wall-7		312	0.6
Wall-8		1305	0.5
Wall-9		Temp profile t	0.6
Wall-10		1100	0.5
Wall-11		1273	0.6
Wall-12		1173	0.6
Wall-13		1173	0.6

H. Solution

Solver is given 1000 no. Of iteration for converging the model.

VI. RESULTS

Our main aim in this study is to simulate the Liquid hydrocarbons for industrial furnaces according to their energy, emissions and availability. We compare between Pentane, Hexane and Heptane. We will determine the correlation between the simulation model and physical combustion process. We are about to investigate for these fuels in combustion at some standard conditions and then investigate emissions contains like CO_x . With this study, we will suggest better fuel for industrial furnaces on the maximum energy, lesser emissions and cheaper cost. In present days, a big challenge is the energy sources because they are non-renewable energy sources.

After the simulation process done in CFD the following results are found. Results of simulation gives a comparison between Pentane , Hexane and Heptane are shown in contour images, which are listed below.

A. Results of PENTANE

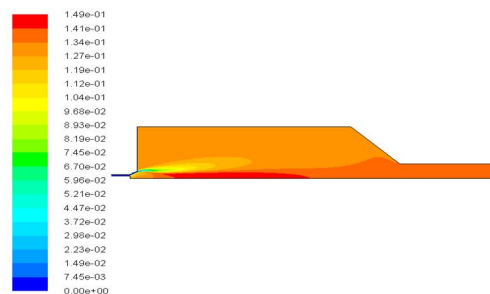


Figure 6.1 Mass Fraction of CO_2

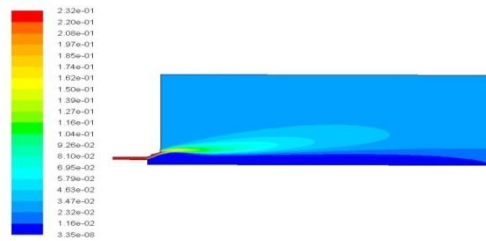


Figure 6.2 Mass Fraction of O2

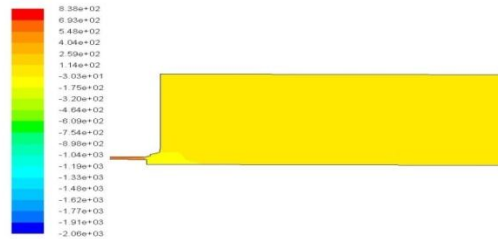


Figure 6.3 Static Pressure

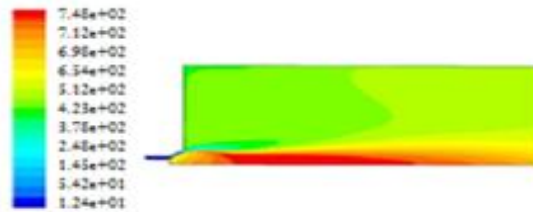


Figure 6.4 Static Temp

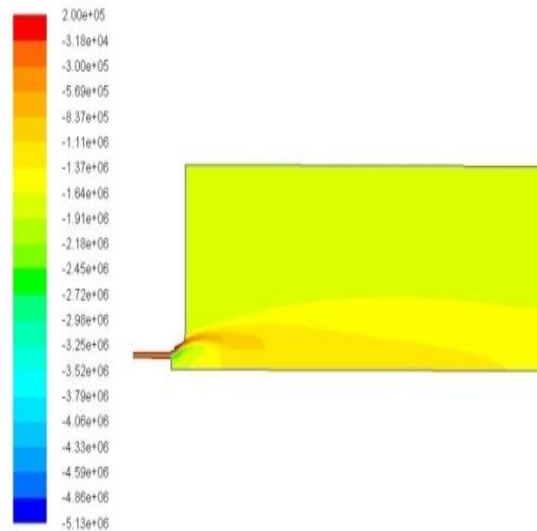


Figure 6.5 Total Energy

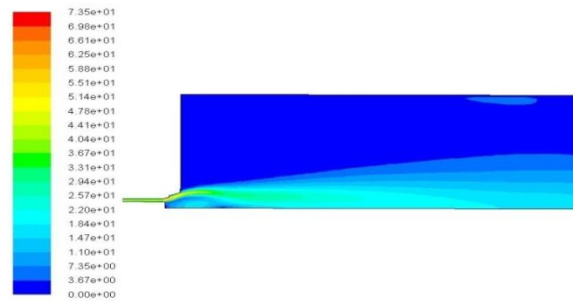


Figure 6.6 Velocity Magnitude

Results of HXANE (Liquid fuel)

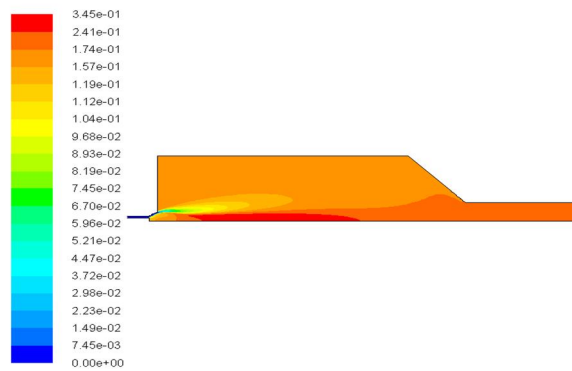


Figure 6.7 Mass Fraction of Co2

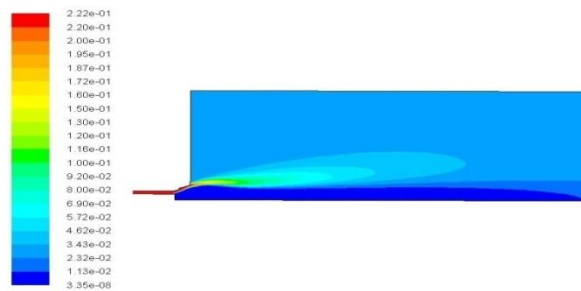


Figure: 6.8 Mass Fraction of O2

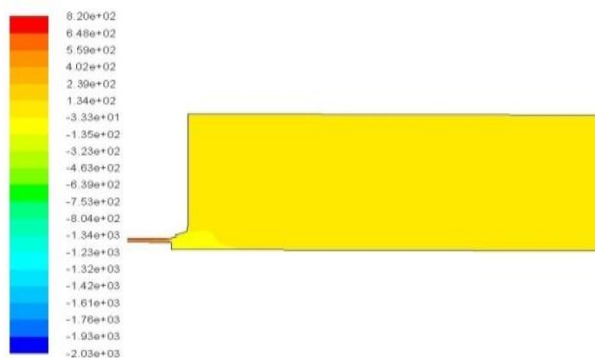


Figure 6.9 Static Temperature

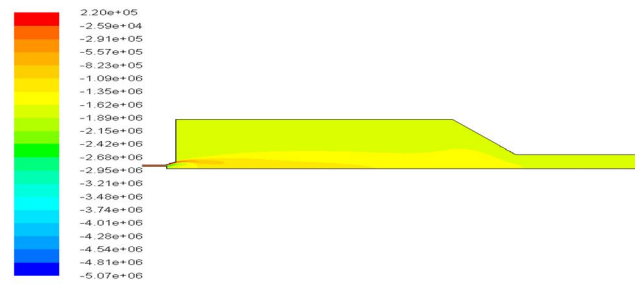


Figure 6.10 Total Energy

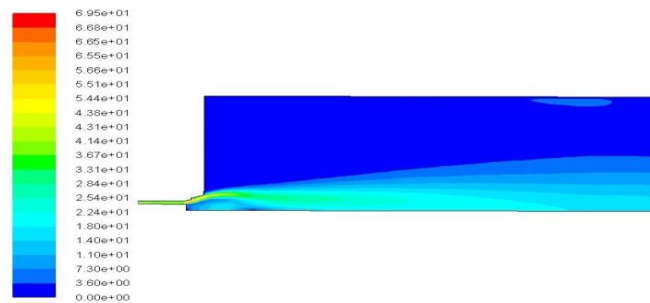


Figure 6.11 Velocity Magnitude

Results of HEPTANE

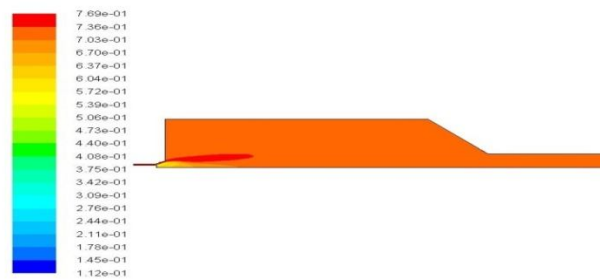


Figure : 6.12 Mass Fraction of Co2

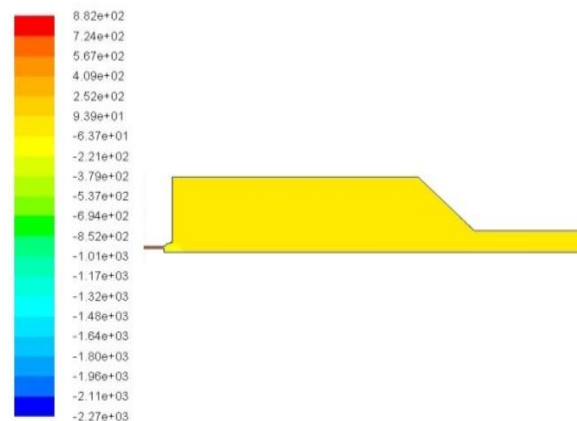


Figure 6.13 Static Temperature

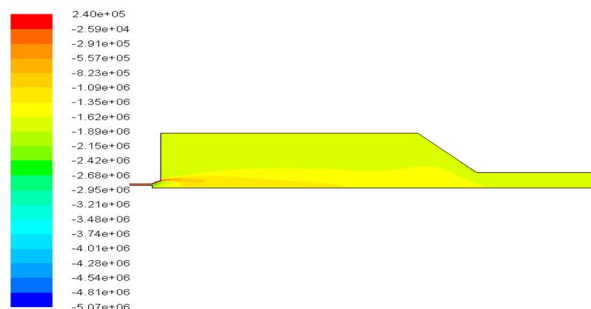


Figure 6.14 Total Energy

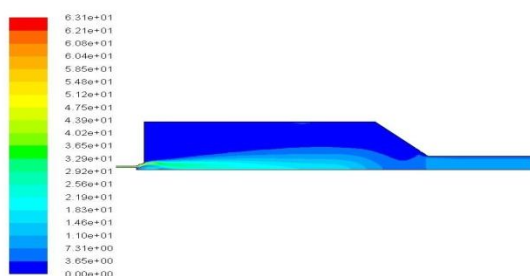


Figure 6.15 Velocity Magnitude

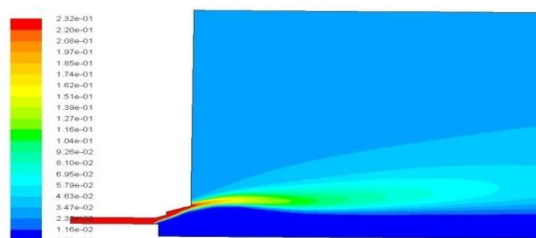


Figure 6.16 Mass Fraction of O2

RESULTS TABLE 6.1

FUEL	TEMPERATURE (K)	TOTAL ENERGY (J/KG)	MASS FRACTION (CO2)	Velocity (m/s)
PENTANE	7.48e+02	2.0e+05	1.49e-01	7.35e+01
HEXANE	8.20e+02	2.2e+05	3.45e-01	6.95e+01
HEPTANE	8.82e+02	2.4e+05	7.69e-01	6.31e+01

VII. CONCLUSION

In this study we compared the simulation results of liquid fuels Pentane, Hexane and Heptane for industrial furnaces. We investigate in this study by the results like Temperature, Total energy, mass fraction of CO₂, turbulence kinetic energy and pressure. By considering different parameters and boundary condition for simulation on ANSYS fluent. We get the results of different physical

values and contour images. According to the results we see total energy and temperature of heptane is the greater one with respect to others. Mass fraction of CO₂ is lesser in Heptane compare to other. We also see the total energy is greater and emission is lesser than pentane. We know that cost is also very low of liquid fuels as compare to low hydrocarbon fuels. Naphthas are a general name given to the C5 - C7 hydrocarbons. These may be found in a variety of solvents for paint, paint thinners, and Bar-B-Q lighter fluids. These are easily vaporized and highly combustible. Liquid fuels or high hydrocarbon have a great advantages over other low carbon fuels because they are in liquid form so that they are easily vaporized in combustion process and there is no need for compressing the fuels.

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