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CFD Modeling of Natural Gas under Different Operating Condition

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Abstract **- In the past decades, natural gas has been, sharply, used as an alternative fuel in industrial sector, power generating system, furnace and various type of burner. Natural gas has higher heating value, low emission and low price in comparison to other fossil fuel. Combustion of various type of fuel (solid liquid and gas) has been studied for a long time. However, because of complex essence of combustion which is a combination of different physical and chemical phenomena, where are still a lot of work should be developed to improve combustion efficiency of thermal system such as burners. In current paper, laminar flame of natural gas produce by "Iraq, Saudi Arabia, Iran, Turkey, Indonesia and China" have been studied in a freely propagation combustion tube. Numerical calculation of laminar flame speed, flame temperature and heat released were performed based on one dimensional model using CHEMKIN PRO.**

Results show that the highest flame speed occurs at an equivalence ratio range of 0.95 and 1.05.Simlar pattern is observed for flame temperature .This means that both laminar flame speed and flame temperature are peak of an equivalence ratio of 1.0.However, the effect of initial pressure on the combustion the natural gas- air mixture on flame speed, flame temperature and heat is observed to be opposite to that accursed of equivalence ratio. Moreover, the effect of initial temperature is quite positive. Since the flame speed, flame temperature and heat released increases. All obtained results show good agreement with other researchers.

Keywords: Natural gas, Laminar flame speed, Carbon monoxide, Oxides of nitrogen.

1. Introduction

Combustion can be defined of a rapid chemical reaction between fuel and air (oxygen O_2) usually a companied by flame and heat released and classified as exothermic reaction. In any combustion application the flame speed play a primary role in understanding this phenomenon. Natural gas is mainly consisting of methane (90% or more) and a trace of other carbon compounds. However, methane has less carbon-hydrogen bond in comparison to the other hydrocarbon fuels, hence; its combustion would not produce soot and can be classified as a clean fuel [1].

Londoño, L. F. et al [2] carried experimental measurement of laminar flame speed for premixed methane –air mixture for different equivalence ratio at sub-atmospheric conditions 852 mbar and 298 K. the authors claim that , the decreasing pressure from 1.013 bar generate an increase of 7% in the laminar flame speed.

CHO, Haeng-Muk; HE, Bang-Quan [3]: studied the combustion and emission characteristics on natural gas engine at MBT spark timings and two fuel injection timings. The researcher had found that the late fuel injection timings can reduce CO and hydrocarbon emissions. But engine NOx emissions can be reduced only at late fuel injection timing conditions. Xuna, Lian, et al.[4]: performed a work to study laminar flame speed of methane-air at various operating conditions including equivalence ratio and initial pressure. The obtained result by the author showed that the laminar flame speed is maximum around the stoichiometric air – methane mixture, but when the initial pressure increase, the laminar flame speed decrease

Dirrenberger, P.et al [5] carried out new experimental measurements of the laminar flame velocity of component of natural gas, methane, ethane, propane and n-butane. The measurements have been performed by the heat flux method using newly built flat flame adiabatic burner at atmospheric pressure. A wide range of equivalence ratio from 0.6 to 2.1 was used. The researcher claims that the results achieved are satisfactory comparing to other studies.

Gianetti1.et al [6] performed a work to find a CDF methodology for the combustion modeling of natural gas for light-duty spark ignition engine. Their results are presented in term of pressure, heat released rate and gross indicated work which show that the methodology can with satisfactory results.

Min Hu [7] presents a numerical modeling of natural gas combustion in order to investigate the behavior of combustion. The numerical model was focus on physical condition, temperature, pressure and equivalence ratio. The researcher used CHEMKIN for his model and the obtained results show good agreement with experiment data.

Salem, Essa KH.[8]carried out a numerical simulation of premixed flame for several the equivalence ratio (lean to rich) and adding a small amount of hydrogen into the fuel blend. Results show an increase of burning velocity and a reduction in NO_x and CO_2.

Liao SY, Jiang Q [9] performed a numerical simulation to determine the laminar flame speed for natural gas. Gülder, Ö. L. [10], carried an experimental work to assess the burning velocity of ethanol –air and ethanol –water-air mixture .the purpose of this study to investigate the laminar flame speed over a wide range of operating conditions including equivalence ratio, initial pressure and temperature.

2. Modeling and Governing Equation

Over the past of 25 years, computer hardware and software have been advanced significantly which make numerical simulation a very competitive tool and particular in engineering field. CHEMKIN PRO is one of software which can be used in current study to facilitate the solution of chemical kinetic problems. It character, a wide variety of flame simulation and reactor model including natural gas laminar flame speed. CHEMKIN PRO includes an extensive library of gas-phase kinetic, surface kinetics, gas transport and thermodynamics data.[11]

Governing equations for freely combustion tube are based on conservation of mass, conservation of energy and species. However, chemical species is generated within the burner would be considered. One dimensional flow with uniform inlet condition will be considered.

1. The mass conservation can be printed as follows:

$$= \rho\, v\, A \;\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. \qquad [1\text{-}a]$$

Where ρ *is* density, v is velocity and A is area.

Or

$$m^{\circ}\,(y_s^{\circ} - y_s^{i}\,) - w_r^{i} V\, M_s^{\circ} = 0 \;\ldots\ldots\ldots \qquad [1\text{-}b]$$

Wherem°: is the total mass flow rate of the fuel and mixture and

$y_s^{\circ} and y_s^{i}$ are the inlet and outlet mass fractions respectively.

w_r°: is the molar rate of production of species S per unit volume.

V : is the volume of burner

M_s°: is the molecular weight of species

2. Conservation of energy

$$M_s^{\circ} \textstyle\sum_{s=1}^{N} \quad (y_s^{\circ} h_s^{\circ} - y_s^{i} h_s^{i}\,) + Q^{\cdot} = 0 \;\ldots\ldots\ldots\ldots\ldots\ldots \quad 2 \quad [11]$$

Where: h_s° *and* $h_s^{i}$are the inlet and outlet specific enthalpies of species respectively.

$Q^{\cdot}$: Heat losses from the burner.

3. Equation of state

$$\rho = \frac{PM^{\cdot}}{RT} \;\ldots\ldots\ldots\ldots.. \qquad 3$$

Where ρ is density, P is pressure, $M^{\cdot}$is Mass, R is constant value for gas and T is temperature.

The density can be determined from the perfect gas equation of state, equation (3), as well as the pressure. The system of equation would be solved using Chemkin pro code named ANSYS.

The laminar flame speed experimental correlation of function of equivalence ratio, pressure and temperate are required to be introduce. Various from of empirical and semi-empirical relationship have been proposed for calculating flame speed [12]. The most widely empirical equation is used:

$$S_L = (B_m + B_{\emptyset}\,(\emptyset - \emptyset_m)^2)(\tfrac{T_u}{T_o})^{\alpha}(\tfrac{P_u}{P_o})^{\beta} \;\ldots\ldots\ldots\ldots.. \quad 4\ [12]$$

Where, *SL* is the laminar flame speed,B_m is the maximum laminar flame speed propagating through thefuel/air mixture at a pressure of 1 atm and a temperature of 300K, $B_{\emptyset}$is the laminar speed roll-off valueused to describe the decay profile of the flame speed from its maximum value, $\emptyset$ is the equivalence ratio, $\emptyset_m$ is the equivalence ratio at maximum laminar speed, *Tu* is the temperature of the unburned gas, $T_o$is the reference temperature of 300 K, $P_u$denotes pressure and $P_o$is the referencepressure of 1 atm. α and β represent the temperature and pressure exponents respectively.

3. Results and Discussion

The laminar flame speed of natural gas-air combustion as function of equivalence ratio (Φ=0.7-1.2) is show in figure (1). It can be seen that the laminar is peak at an equivalence ratio of 1.02 for all used natural gas. Figure (2) show the relationship between flame speed and initial pressure at an equivalence ratio of 1.0, while the initial temperate is kept constant at 298 $\approx$ 300 K. It can be noted that the flame speed decrease gradually as the initial pressure increase. The effect of initial temperate on laminar flame speed is pictured in figure (3). It can be observed that the flame speed increases as the initial temperature increase. Figure (4) show the relationship between flame temperature and equivalence ratio , which 0.7 – 1.2 for all types of natural gas it can be seen that flame temperate have maximum value , nearly at an equivalence around1.0. Figure (5) show the relationship between the flame temperature and initial pressure of the natural gas-air mixture at an equivalence ratio of $\emptyset \approx 1.0$. It can be seen that the initial pressure has a positive effect on flame temperature for all considered fuel (Iraq, Saudi Arabia, Iran, Turkey, Indonesia , China). Moreover, the Indonesia natural gas shows the highest flame temperature among other. Iraqi nature gas flame temperature show little reduction in comparison with Indonesia natural gas. The chemical composition for each investigated natural gas is given in table 1[13,14,15,16].

The effect of initial temperate of the mixture on the flame temperature is pictured in figure (6). It can be noted that the flame temperate increase sharply as the initial temperature increase. Combustion of natural gas-air mixture for an equivalence over range (Ø=0.7-1.2) at (T=300 K) and pressure 1 atm for various type of fuel is given in figure (7).

Examining the figure, it can be seen that the max heat released occur at equivalence ratio approximately $(\emptyset \approx 1.0)$. This because all carbon curveted to CO_2 and all H_2O converted to $H_2O_{(v)}$and no oxygen diluted the flame.

Figure (8) and (9): show the effect of initial pressure and initial temperature on the head released. Both parameters have appositive effect. Mole fraction of NO_x produced during the combustion of natural gas-air mixture are obtain by changing the equivalence ratio (Ø=0.7-1.2) for a constant reactants inlet temperature (T=300 K) and a constant reactants inlet pressure (P=1atm) as shown in figure (10). It can be seen that maximum formation occurs at (Ø=0.96) because flame temperature is quite high at (Ø=0.96) , while for lean and rich mixture, the formation of NO_xwill be quite low. Figure (11) show the formation of CO for all considered fuel from (Ø=0.7-1.2). It can be observed that the highest level of CO are generated through the combustion of natural gas at (Ø>1.0) rich mixture. This may be explanted as Ø>1.0, then there is no enough oxygen to convert all carbon to CO_2 , hence, carbon monoxides CO will be present. All gathered result has an experimental and theatrical validation with other researchers.

4. Conclusion

The conclusion of current study can be summarized as follows:

1. The maximum flame speed for combustion of natural gas- air mixture occurs nearly at Ø≈1.0 for all considered natural gas.
2. The laminar flame speed for Iraqi natural gas show the maximum value of 40.4 cm/ sec.
3. The laminar flame speed for natural gas- air mixture increase linearly with the increase in initial temperature for lean ,stoichiometric and rich mixture.
4. As the initial pressure increase, the laminar flame speed would decrease for lean, stoichiometric and rich mixture.
5. The increase in initial pressure led to increase in flame temperature, but flame speed decreased.
6. The heat released increase as the initial temperature and pressure increase, for all mixture strength.
7. The emission of carbon monoxide decrease for lean mixture (Ø<1.0) and increase for rich mixture (Ø>1.0), because a shortage of oxygen present in rich mixture. However, the emission of NO_x peak at stoichiometric mixture, due to high temperature.

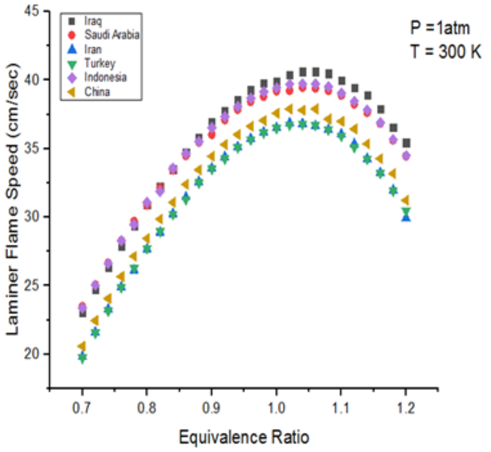

Figure 1: Natural gas laminar flame speed at different equivalence ratios

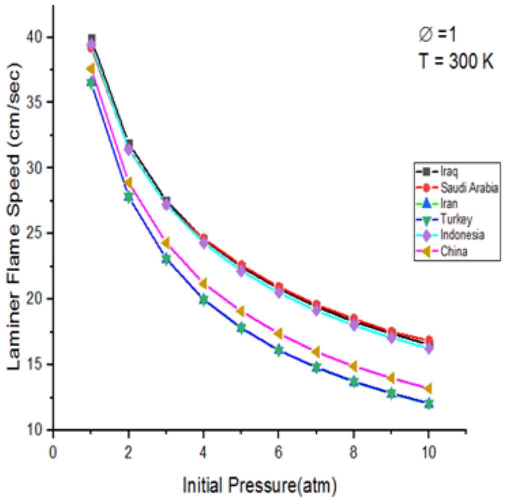

Figure 2: Natural gas laminar flame speed at different initial pressure

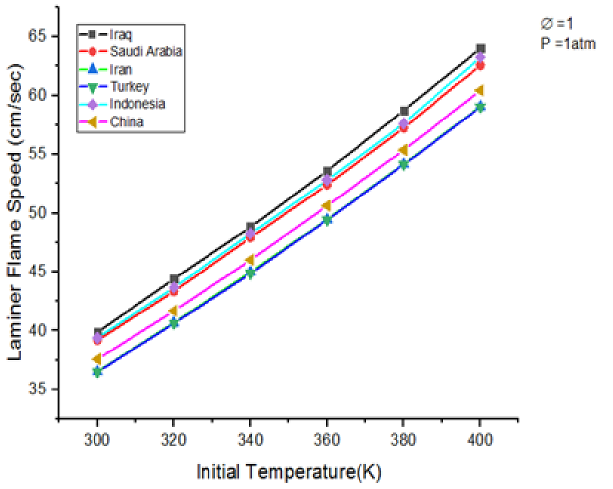

Figure 3: Natural gas laminar flame speed at different initial temperature

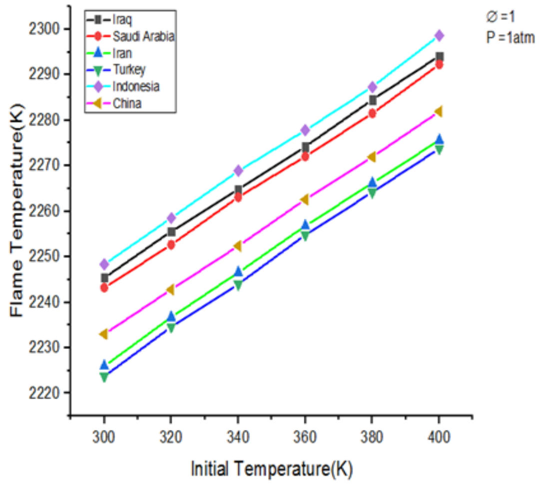

Figure 6: Natural gas flame temperature at different initial temperature

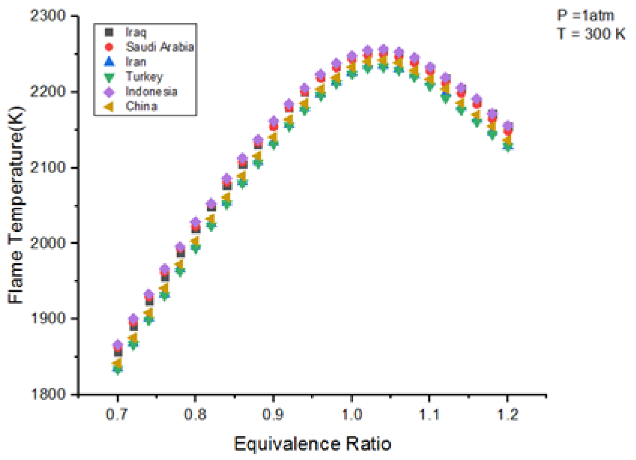

Figure 4: Natural gas flame temperature at different equivalence ratios

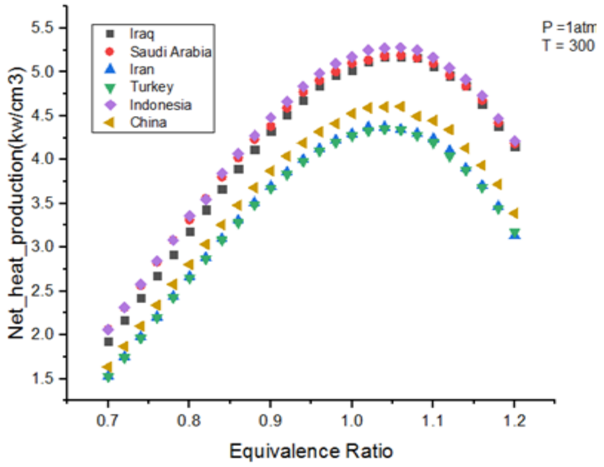

Figure 7: Natural gas net heat production at different equivalence ratios

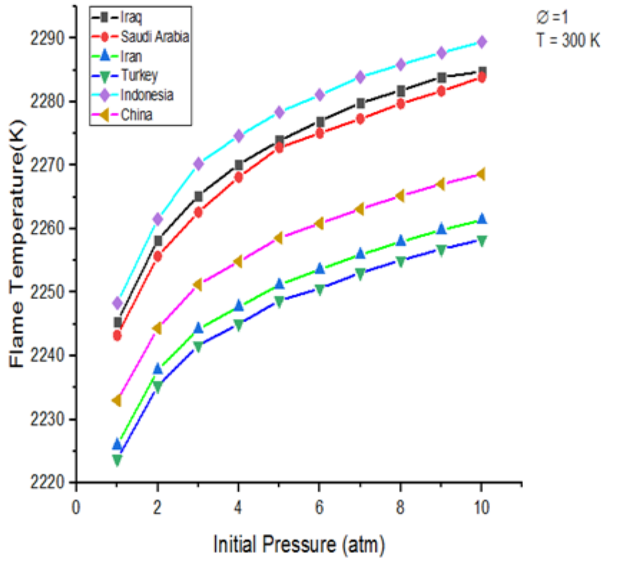

Figure 5: Natural gas flame temperature at different initial pressure

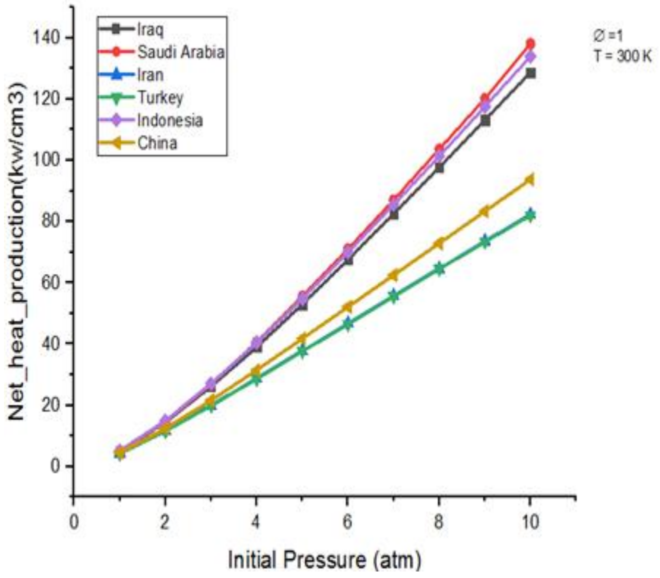

Figure 8: Natural gas net heat production at different initial pressure

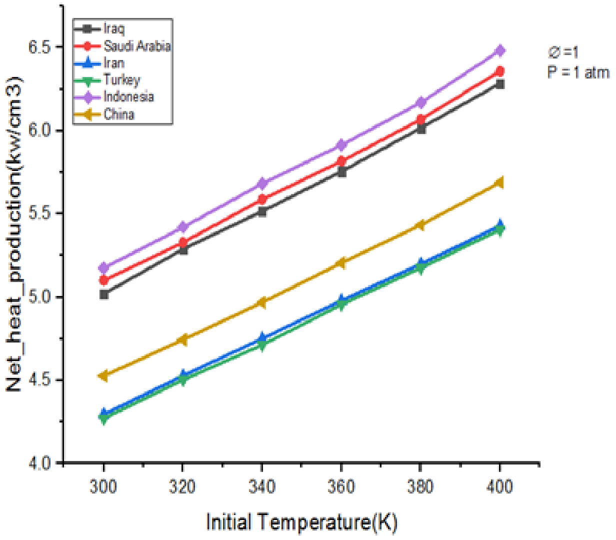

Figure 9: Natural gas net heat production at different initial temperature

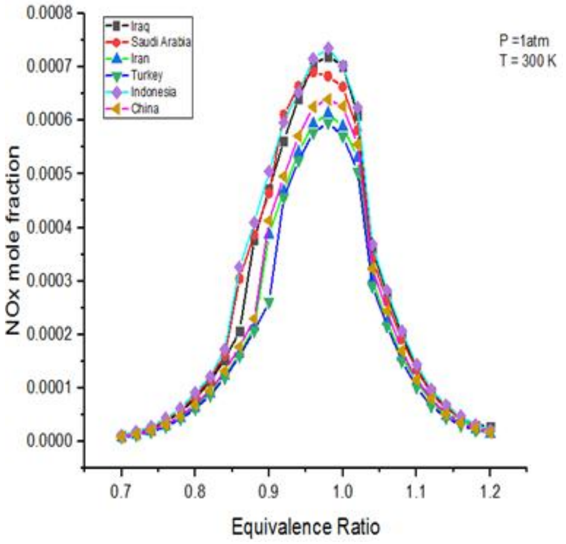

Figure 10: Natural gas NO_x mole fraction at different equivalence ratios

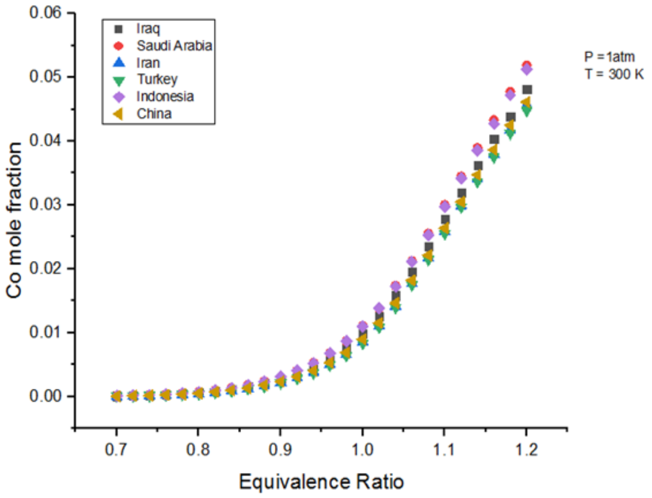

Figure 11: CO mole fraction at different equivalence ratios

Table 1: Composition of different natural gases

	Iraq	Saudi Arabia	Iran	Turkey	Indonesia	China
CH_4	76.47	69.01	97.4	92.6	65.7	92.59
C_2H_6	22.28	5.7	-	0.5	8.5	3.19
C_3H_8	0.14	2.3	-	0.1	14.5	1.36
C_4H_{10}	1,08	1.21	-	-	5.1	0.34
C_5H_{12}	-	0.9	-	-	0.8	-
H_2S	-	5.02	-	-	-	-
CO_2	-	3.46	2.1	0.1	4.1	0.93
N_2	0.03	12.4	-	6.4	1.3	1.59
Others Composition	-	-	0.5	0.3	-	-

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