Investigation of Influencing Parameters and Determination of the Lower and Upper Limits of Flammability of a 25MW Industrial Gas Turbine Combustor

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ABSTRACT

In the paper, combustion flammability limits in the combustion chamber of gas turbines and effective factors on these limits would be studied. Considering flammability, initiation of combustion and stability limit are very important parameters in the performance of the gas turbine combustion chamber and to study these factors, flammability of combustion has to be controlled. So, in the paper, the method of calculation of these limits and factors having effects on them would be studied. Also, some of the theoretical models would be reviewed, in which flammability limits would be estimated through experimental data. Finally, with consideration of the aforementioned relations, an optimal method for calculation of upper and lower flammability limits in the gas turbine combustion chamber would be presented.

KeyWords: *Combustion Chamber, Gas Turbine, Upper Flammability Limit (UFL), Lower Flammability Limit (LFL)*

Introduction

Gas Turbines are one of the important devices for generation of the power and electricity. A compressed air is generated through the compressor [1] and its pressure is increased within the diffuser [2]. Then, the high pressure, low speed air is mixed with fuel and burnt in the combustor and provides mechanical energy in the turbine which will be used for power or electricity generation. If a very little fuel in the form of gas or vapor would be added to the air in the vicinity of sparkle or flame, the fuel would not become inflamed. However, if the amount of fuel would be increased, inflammation would be taken place in a certain percentage of fuel ratio to air. This limit is called the lower flammability limit. The more would become the amount of fuel, the more intensified would become combustion (burning) process so that it reaches to its maximum level. Thereafter, an increasing percentage of fuel would result in a reduction of combustion intensity so that no more combustion would be taken place. This percentage is called the upper flammability limit [3]. In brief, flammability limits are in two kinds:

1. Upper flammability limit: Where fuel density for inflammation is too high;
2. Lower flammability limit: Where fuel density is too low to make a sparkle.

Usually, flammability limits would be calculated through empirical tests in which inflammation limits of various mixtures of air-fuel would be specified. Following relationship is one of the equations based on which empirical calculations of flammability limits are performed [4].

$$LFL_{T,P} = \frac{1}{2}\left(C_{g,n} + C_{l,f}\right) \tag{1}$$

$$UFL_{T,P} = \frac{1}{2}\left(C_{g,f} + C_{l,n}\right) \tag{2}$$

Where, $LFL_{T,p}$, and $UFL_{T,P}$ are respectively lower and upper flammability limits under certain temperature and pressure. $C_{g,n,}$ and $C_{l,n}$ are respectively maximum and minimum fuel concentrations in the non-combustible oxidizer. $C_{g,f}$ and $C_{l,f}$ are respectively maximum and minimum fuel concentrations in combustible oxidizer [5]. Practically, flammability limits of a certain system of fuel and air are affected by different factors such as temperature, pressure, oxygen concentration, neutral gas concentration, size of equipment, the direction of flame propagation, flow turbulence, gravitational field, and etc. In continuation, some of the effective factors on flammability limits would be discussed and reviewed.

Effect of Temperature on Flammability

One of the effective factors in the calculation range of flammability is the thermal condition. That is, an increase or decrease of temperature considerably affects flammability limits of the mixture of gases. In 1965, through research performed on combustible gases and steam by Zabetakis [6], the emphasis has been put on the point that flammability limits of most of the fuels will not remain fixed in various temperatures at the outlet of the combustion chamber. Especially, when outlet temperature increases, lower and upper flammability limits would be decreased and increased, respectively. In industrial applications, sometimes some of the air-fuel mixtures remain aflame; however, they remain outside flammability limits. Effects of temperature change on flammability limits are shown in Figure (1).

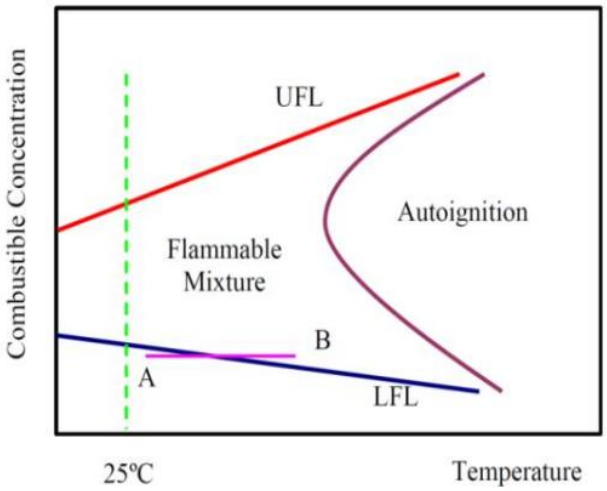

Figure 1. Effects of temperature change on flammability limits (Zabetakis, 1965 [6])

As it was observed by Zabetakis et al. (1951), in most of the hydrocarbons, LFL will show 8% reduction against each 100˚C increase in the mixture's temperature. Considering the researches performed by Bureau of Mines (BM) [6], with certain LFL value specified in room temperature (25˚C); it could be calculated in another temperature according to a relationship (3). Equation (4) also has been proposed by BM to compute UFL, through temperature increase.

$$\frac{LFL_{T_2}}{LFL_{25}} = 1 - 0.000784\left(T_2 - 25\right) \tag{3}$$

$$\frac{UFL_{T_2}}{UFL_{25}} = 1 + 0.000721\left(T_2 - 25\right) \tag{4}$$

Later, above relationships have been modified and presented as relationships (5) and (6) by Burgess-Wheeler in relation to the effect of temperature on LFL and UFL of hydrocarbons, in

absence of cool flame (flammable mixture of fuel and air in which flame is created upon maximum 700K temperature which is not visible by eyes even in the light) [8].

$$LFL_T = LFL_{25} - \frac{0.75}{\Delta H_C}(T - 25) \quad (5)$$

$$UFL_T = UFL_{25} + \frac{0.75}{\Delta H_C}(T - 25) \quad (6)$$

Where ΔH_C is net heat resulted from combustion (Kcal/mole). Considering the above equations, it could be found that temperature increase will lead to an increase of UFL and decrease of LFL; and, briefly speaking, flammability range would be increased.

Effect of Pressure on Flammability Limits

Usually, pressure has a minor effect on LFL, except for in low levels (lower than absolute pressure=50mmHg); however, UFL would be considerably increased through increase made in pressure. The flame temperature has been calculated as a function of density and pressure, by Melhem [7] for different gases. As observed by him, pressure increase causes an increase in temperature for rich fuel mixtures; however, it has no effect on lean mixtures.

$$LFL_P = LFL_{1atm} - 0.31 \ln P \quad (7)$$

$$UFL_P = UFL_{1atm} + 8.9 \ln P \quad (8)$$

Relationships related to changes of UFL and LFL according to pressure are consistent with relationships (7) and (8) [7].

Therefore, if the flame temperature in the flammability limits would be fixed, UFL would be increased through an increase of pressure; however, no change would be made in LFL. Figure (2) shows the effects of initial pressure on flammability limits of natural gas.

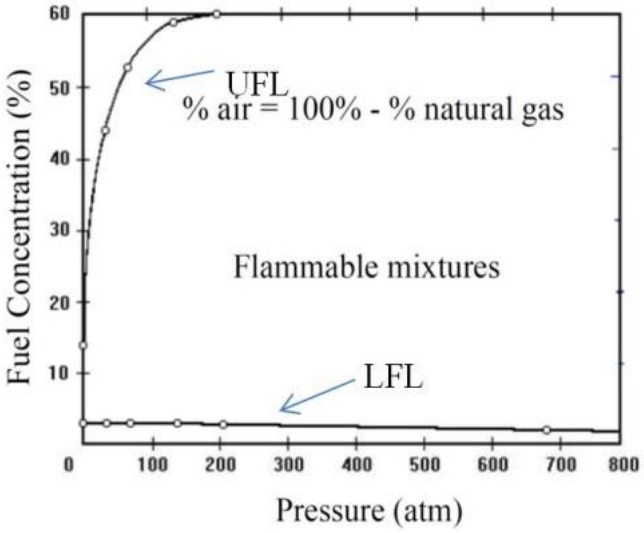

Figure 2. Effects of pressure on flammability limits of natural gas in 28˚C (Zabetakis, 1965 [6])

As shown in Figure (2), LFL would be reduced through a minimal increase in pressure; however, UFL changes would be high. The reason is the direct relationship between pressure and chemical reaction mechanism. Since in chemical mechanism of combining fuel and oxidizer in rich fuel mixtures, burning rate is directly related to pressure in reaction mechanism and pressure changes are exponential; only UFL would be considerably increased through an increase in pressure. Also, with consideration of figure (3) that shows pressure effect on flammability limit of methane gas presented by Shigeo Kondo (2011) [9]; the linear relationship of pressure and increase of UFL is observed which is contrary to the results provided by other researchers. According to figure (3), it is also observed that in upper flammability limit when pressure increases within certain pressure range; a sudden increase would be observed in UFL which will be continued to a certain level of pressure. Thereafter, an increasing trend of flammability limit will be adjusted through an increase in pressure. The reason could be a change in combustion reaction mechanism in these two upper flammability limits which are under 1000kPa and over 1500kPa for methane (figure 3).

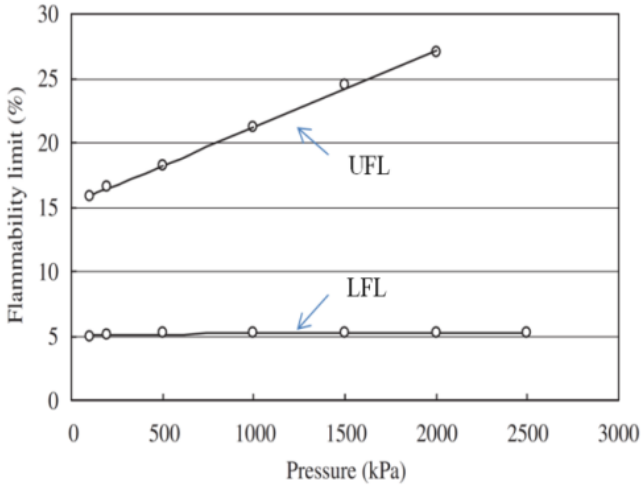

Figure 3. Effect of pressure on methane gas flammability limits

Relationship (9) has been provided by Zabetakis as for the effect of pressure on flammability limits [5].

$$FL(P) = FL(P_0) + C\left(\frac{P}{P_0}\right) \tag{9}$$

Where, FL(P) indicates upper and lower flammability limits under pressure *P*, *FL(P₀)* is certain flammability limits under imposed pressure, and P_0 and *C* are constants equal to -0.71 and 20.4 for lower and upper flammability limits.

Effect of Oxygen Concentration on Flammability Limits

Since LFL concerns lean fuel condition, an increase of oxygen volume concentration up to 21% in the air-fuel mixture is acceptable; and, excessive increase of it only acts as a diluent. Molar heat capacities of oxygen and nitrogen are similar; as a result, LFL will not change through up to 100% increase of oxygen in the atmosphere. However, UFL will be considerably increased through increase made in oxygen concentration. When the oxygen concentration in the air is continuously decreased, LFL and UFL would be convergent at one point; where, oxygen concentration will be reduced to a minimum level (minimum oxygen concentration-MOC). In figure 4, the relationship between flammability limits and changes in oxygen concentration is shown in a system including methane-oxygen-nitrogen [6].

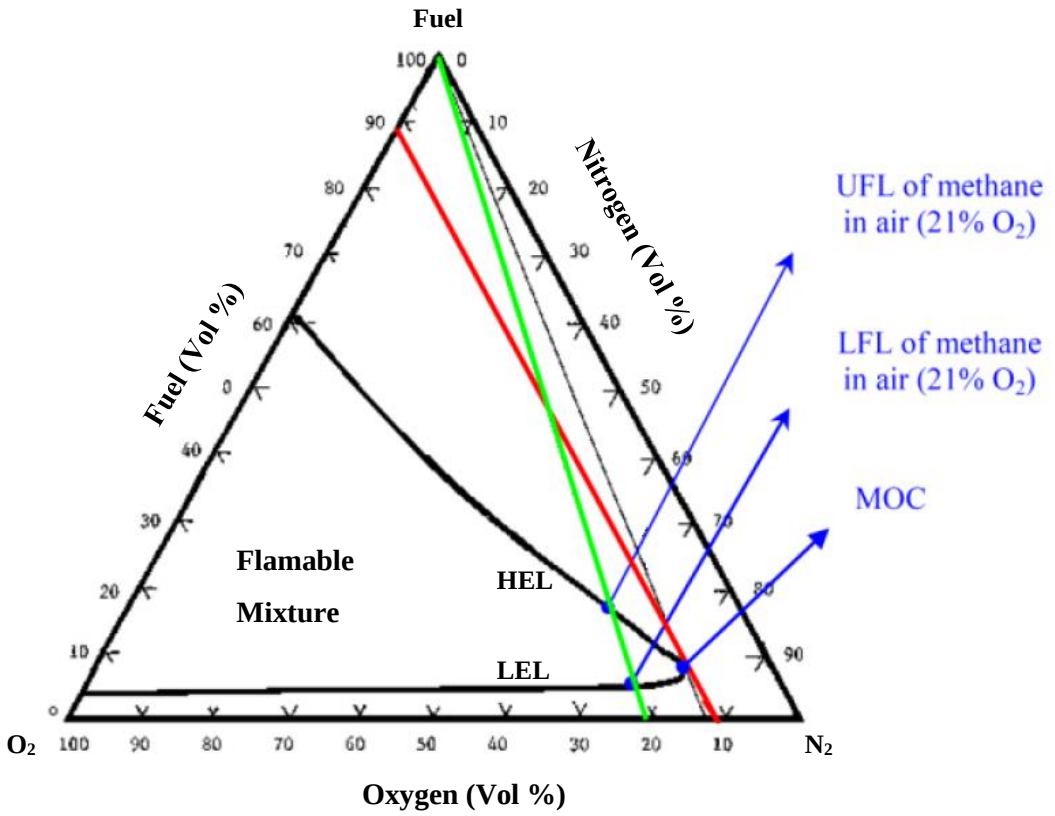

Figure 4. Flammability diagram with changes in oxygen concentration (Zabetakis, 1965 [6])

Effects of Neutral Gases on Flammability Limits

Existence of neutral gases has a considerable effect on the chemical reaction mechanism. Existence of neutral gas during combustion also would be resulted in dilution [3]. In order for combustion or explosion to take place, all flammable materials existing in the air have to have a concentration higher than LFL and lower than UFL. To control combustion and explosion, sometimes neutral additive gases (they are neither fuel nor oxidizer) would be added to the mixture to reduce flammability limits of the reaction mixture, or taking it out from these limits. Effects of neutral gases on flammability limits have been comprehensively studied by Besnard [9]. A number of neutral gases with various inactivating capacities have been studied by him as for reduction of flammability limits of air-fuel mixtures. Figure (5) shows related lab results in which changes of methane flammability limits in air and under standard condition are shown, at the presence of added neutral gases [9].

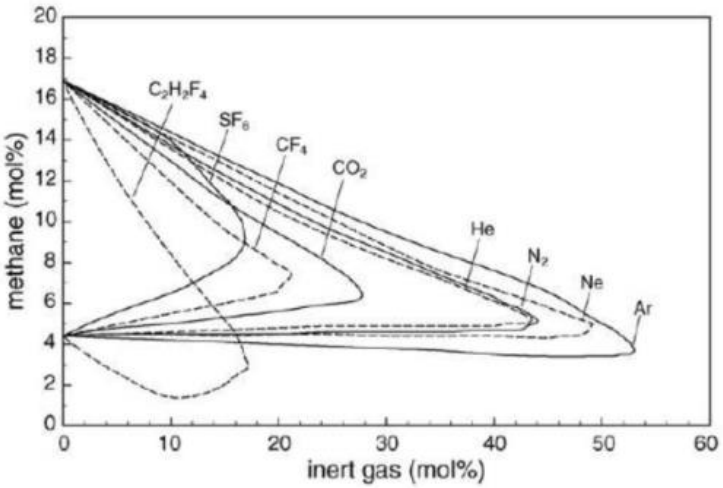

Figure 5. Effect of neutral gases on Methane flammability limits in the air (Besnard, 1996 [9])

According to the figure (5), average amounts of neutral gases mainly affect UFL (except for $C_2H_2F_4$). If enough amount of neutral gas would be added to the mixture, all of them are capable of turning the mixture to a non-combustible one [4].

Effect of Lab Equipment on Flammability Limits

It has been about 200 years since flammability limits have been measured with different devices through lab operations. So, the results have shown that the size of lab equipment applied is dependent on flammability limits. A vertical cylindrical tube with 5cm in diameter has been used by Coward and Jones [10] as for measurement of flammability limits of various gases. Later, Zabetakis suggested that using a tube with 5cm diameter is very small for measurement of hydrocarbon's flammability limits. The results from a comprehensive research performed on flammability changes through changes of size and shape of the vessel could be summarized as follows: 1- For cylindrical tubes with low diameter and high height, flammability limits are basically determined by effects of wall cooling; 2- for low height cylindrical tubes, flammability limits would be calculated as affected by hot gases accumulated at the vessel ceiling, heat of unburned gases, automatic heat of initial flame, and effect of cooling the walls; 3- If vessel size would be large enough, all of the aforementioned effects could be ignored; and, experimental value of flammability limits can reach to that of free space [11]. In figure (6), the relationship between methane flammability limits changing through changes made in vessel size is shown.

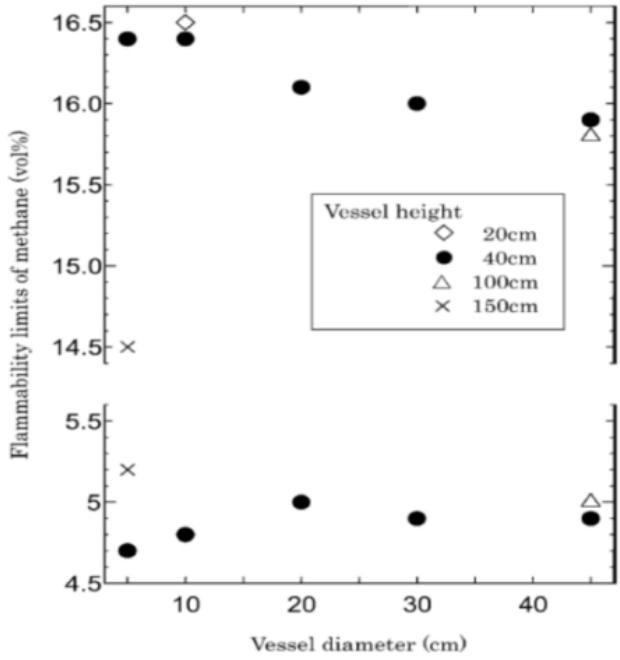

Figure 6. Methane gas flammability limits in various sizes and shapes of vessels (Takahashi, 2003 [11])

Effect of Ignition Energy on Flammability Limits

Gas or steam mixtures require initial ignition energy for combustion. The minimum energy required for the burning of the combustible gas mixture to be started is called minimum ignition energy (MIE). In general, most of the flammable mixtures can burn by relatively low energy ignition (about 1 to 100mJ) [11].

For a mixture of fuel-oxidizer within flammability range, a minimum amount of energy is required for ignition and it is called ignition energy. Also, a concentration range of mixture dependent on ignition power is called ignition limits (figure 6). Ignition energy is dependent on mixture concentration. Figure (7) shows the effect of the mixture's composition on ignition energy required for air-methane mixture to become ignited [12]. A range of mixture concentration which necessarily is independent of the source of ignition and indicates the capability of a flame for propagation from the source of ignition is called flammability limits. Very high amount of ignition energy is required to maintain flammability limits, compared to the energy required for ignition limits. Also, more energy is usually required for UFL to be established, compared to LFL.

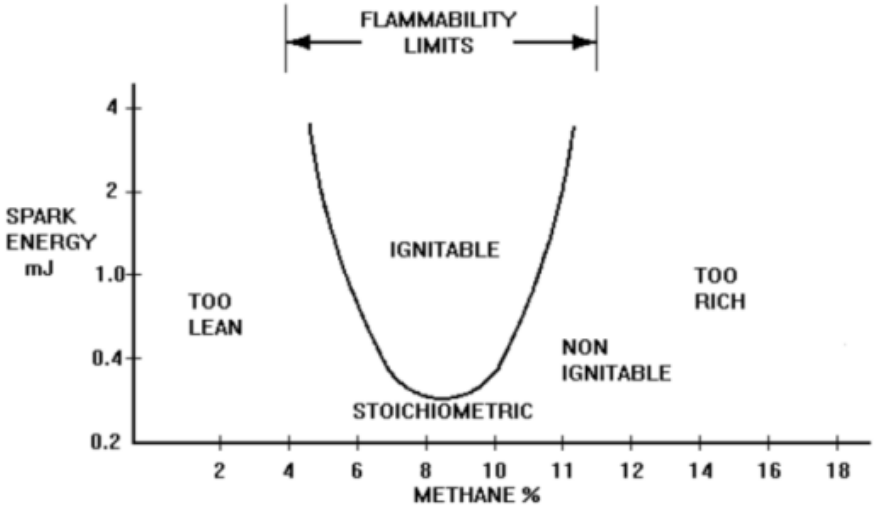

Figure 7. Sparkle curve and flammability limits for a mixture of air/methane under atmosphere pressure and 26˚C [12]

Effect of Direction of Flow Propagation on Flammability Limits

It has been proved by Clowes and Eitner (1902) [13] that flammability limits for upward flame propagation is wider than that of downward flame propagation. It was shown by Leprince-Ringuet (1914) [14] that, limits for horizontal propagation are between those for upward and downward propagation. Near flammability limit, the flame cannot move downwardly; because, buoyancy force causes an upward flow. Considering table (1) showing the effect of flame propagation direction on flammability limits, it is found that the direction of flame propagation in UFL is more effective than that of LFL.

Table 1- Effect of flame propagation direction on flammability limits (White, 1924) [15]

UFL volume percentage	LFL volume percentage	Propagation direction	Mixture
14.85	5.35	Upward	
13.95	5.40	Horizontal	Methane/air
13.35	5.95	Downward	
8.0	1.42	Upward	
7.45	1.44	Horizontal	Pentane/air
4.64	1.48	Downward	
7.45	1.45	Upward	
6.65	1.46	Horizontal	Benzene/air
5.55	1.48	downward	

Estimated Modeling of Flammability Limits

Despite the fact that lab data are always required for calculation of flammability limits, some researchers have provided theoretical relationships to compute flammability limits, through experimental data. For example, flammability limits are calculated through Shimy equations [16], based on atoms existing in fuel.

Shimy Equations

Several empirical equations have been presented by Shimy as for estimation of upper and lower flammability limits of various chemical elements under atmosphere pressure and room temperature. The results are shown in table (2).

Table 2- Shimy equations to estimate flammability limits under standard condition (Shimy, A.A., 1970 [16])

	LFL	**UFL**
Paraffinic Hydrocarbons and Olefins	$\frac{6}{nC^a}+0.2$	$\frac{60}{nH^a}+\frac{nC}{20}+2.2$
Iso-Hydrocarbons	$\frac{6}{nC}+0.1$	$\frac{60}{nH}+2.3$
Benzene Series	$\frac{8}{nC}$	$\frac{86}{2nH_r^c+nH'^d}$
Alcohols	$\frac{6}{nC}-0.7$	$\frac{80-2nH}{2nC}+3$

In table 2, nC is a number of carbon atoms, nH is the number of hydrogen atoms, nHr is a number of hydrogen radical atoms, and nH' is number of non-radical atoms of hydrogen.

In Shimy equations, lower flammability limit is just a function of the number of carbon atoms; whereas, upper flammability limit is related to the number of carbon atoms, and hydrogen radical and non-radical atoms.

Modeling through Calculated Adiabatic Flame Temperature

Since the adiabatic flame temperature in following paraffin (paraffin are saturated hydrocarbon compounds called alkanes in which all carbon atoms existing in the molecule are bound to each other through singe bonds. In other words, paraffin hydrocarbons are featured by single bonds between carbon atoms, and their general formula is C_nH_{2n+2}) almost remains fixed; some of the researchers have used the issue to estimate flammability limits. Nowadays, CAFT (*calculation* of adiabatic flame temperatures) method is a powerful tool to estimate the lower flammability limit of gas mixtures. To estimate flammability limits, a thermal threshold of 1550K, 1200K, and or 1500K has been considered by some groups. In continuation, the method proposed by Shebeko [17] and used for calculation of lower flammability limit would be presented in which adiabatic flame temperature has been supposed to be 1600K, and related relationship is as follows:

$$LFL = \frac{100}{1 + \nu_{a0}} \tag{10}$$

Where, ν_{a0} is the ratio of a number of moles of air to the number of moles of fuel in the mixture and in lower flammability limit.

Writing energy balance equation (11), we will have:

$$\sum_i H_{react,i}(T_i, P) = \sum_i H_{prod,j}(T_{ad}, P) \tag{11}$$

where, $H_{react,\,i}$ and $H_{prod,\,j}$ are enthalpies of reactants and products. T_i is initial temperature and T_{ad} is adiabatic flame temperature, also being equal to final temperature [17]. Supposing the fuel as $C_nH_mO_1$ that makes reaction with air, and through placement and simplification of the above equation, finally for lower flammability limit, it will be:

$$LFL = \frac{100}{1 + g_f \Delta H_f + g_C n + g_H m + g_O l} \tag{12}$$

Where:

$$\begin{cases} g_f = \dfrac{1}{H_a^{ad} - H_a^i} \qquad g_C = g_f\left(H_C^i - H_{CO2}^{ad} + H_{O2}^{ad}\right) \\ g_H = 0.5 g_f\left(H_{H2}^i - H_{HO2}^{ad} + 0.5 H_{O2}^{ad}\right) \\ g_O = -0.5 g_f\left(H_{O2}^{ad} - H_{O2}^I\right) \end{cases} \tag{13}$$

Considering the above relationships, the lower flammability limit can be calculated.

Le Chatelier Model

Using lab test results performed for calculation of LFL in the mixture of methane and several other gases, a principle has been obtained by Le Chatelier for calculation of flammability limit of a mixture of gases. Le Chatelier Principle shown as equation (14) is highly applicable and well-known, presented only for LFL calculation of a mixture of gases.

$$LFL_{mix} = \frac{1}{\sum_{i=1}^{N} \frac{y_i}{LFL_i}} \tag{14}$$

Where y_i is the mass fraction of i^{th} gas, LFL_i is flammability limit of i^{th} gas, and LFL_{mix} is LFL of the mixture of gases. Considering Le Chatelier's algebraic relationship, it could be found that LFL of the mixture of gases is a value between the minimum and maximum flammability limits of mixed gases.

Later, Kondo et al. have generalized Le Chatelier principle in the form of equation (15) to estimate the upper flammability limit.

$$UFL_{mix} = \frac{1}{\sum_{i=1}^{N} \frac{y_i}{UFL_i}} \tag{15}$$

Proposed Method to Calculate Flammability Limit in Numerical Model of Gas Turbine Combustion Chamber

In numerical methods and to calculate flammability limits, a one-dimensional surface flame could be solved with consideration of reaction kinetics and/or Arrhenius equation. That is, the problem would be solved for several different equivalence ratios. Firstly, the solving process would be begun with several low equivalence ratios (for lean mixture) till the initiation of flame;

then, LFL would be calculated. The problem would be also solved for several high equivalence ratios so that it would be cleared that what is the maximum fuel concentration corresponding to the equivalence, upon which flame would not be put out. In the present method and using a numerical method, an estimation of flammability limits of the gas mixture has been obtained, primarily. Then, with consideration of quasi-experimental relationships (Le Chatelier equations) and also experimental results more accurate calculation of flammability limits in the gas turbine combustion chamber has been performed (Figure 8). In figure (8), combustion flammability range in the gas turbine combustion chamber under the total temperature of 700K and total pressure of 1000kPa at the inlet with is presented, with methane 100%. Considering the presented equations, our research model can calculate flammability range under various working and thermodynamic conditions and the mixture of air-fuel in various gas turbine stations.

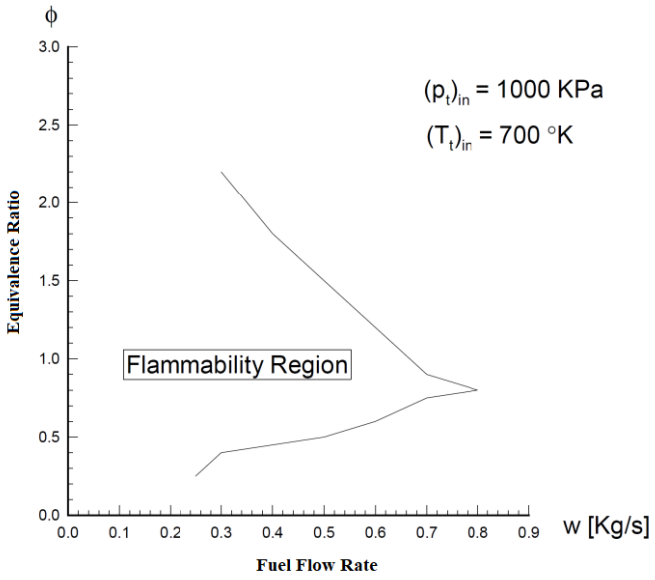

Figure 8. Flammability area obtained for gas turbine combustion chamber in the present proposed model

Conclusion

In the paper, the calculation method of flammability limits and effective factors on upper and lower flammability limits have been studied. As it was observed, the increase in temperature would result in an increase of UFL and decrease of UFL. Also, it was found that increasing pressure will lead to a considerable increase in UFL; whereas, it has a minor effect on LFL. After review of effective factors on flammability range, theoretical models estimating these limits have been studied. Also, with consideration of the above, a mechanism has been provided

as for calculation of flammability limits in numerical simulations. Finally, with consideration of experimental and theoretical data related to the gas turbine combustion chamber, flammability diagram of combustion has been obtained. In the present model and for various types of fuels under different thermodynamic conditions (different pressures and temperatures) in gas turbine station, flammability range could be calculated based on changes in various temperature and pressure ranges.

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