Adiabatic Flame Temperature New Calculation Technique

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Abstract: - The present paper introduces the methane-air flame and its main chemical reaction, the mass burning rate, the burning velocity, and the most important parameter the adiabatic and its evaluation. Those major important flame parameters will be mathematically formulated, and computerized using the MATLAB program. The present program established a new technique to decide the true adiabatic flame temperature, where there are no combustion energy losses to the surrounding also, no shaft work or energy gaining from outside, and all the heat generate from the exothermic reaction will release to their product. The new technique implements the trial, and error procedure to obtained the calculated total internal energy of the product species then evaluate of the reactant's ones, from both we can draw two energy lines their intersection will decide the true required temperature. The obtained result show accurate evaluation to the adiabatic temperature for the atmospheric (P=1.0 atmos) Stoichiometric (Φ =1.05) methane-air flame and was 2136.36 K.

Key-Words: - Methane-Air Flame Stoichiometric Adiabatic flame temperature Reaction model MATLAB Program New technique

1 Introduction

Long times ago the methane gas was discovered and soon becomes one of the major important fuels for both domestic and commercial purposes. It's well knowing that methane has the following chemical formula:



Fig.1. Chemical formula of methane gas molecule.

The availability of the gas and petroleum around the world were widely investigated by a number of organizations and were clearly shown on a map [1]. While its burning in the stoichiometric reaction can be represented by the following chemical formula [2, & 3]:

$$CH_4 + 9.523 (0.21O_2 + 0.76N_2) \stackrel{Q}{\Rightarrow} CO_2 + 2H_2O + 7.237N_2$$
(1)

and has several involved steps. These are:

1- Methane forms to a methyl radical (CH3), which reacts to formaldehyde (HCHO or H2CO). The formaldehyde reacts to a formal radical (HCO), which then forms carbon monoxide (CO) (Eq.2). The process is called oxidative pyrolysis:

$$CH_4 + O_2 \to CO + H_2 + H_2O$$
 (2)

2- Following oxidative Pyrolysis, the H2 oxidizes, forming H2O (Eq.3), replenishing the active species, and releasing heat. This occurs very quickly, usually in less than a millisecond.

$$H_2 + \frac{1}{2}O_2 \to H_2O \tag{3}$$

3- Finally, the CO oxidizes, forming CO2 and releasing more heat (Eq.4). This process is generally slower than the other chemical steps, and typically requires a few to several milliseconds to occur.

$$CO + \frac{1}{2}O_2 \to CO_2 \tag{4}$$

Methane – Air reaction able to generate heat amount of 55.5 MJ/kg (x 238.85 kcal/kg), while the typical scientific properties of the gas are [2, & 3]:

$$\rho_{cH_4} = 0.6589 \text{ kg/m}^3$$
 (At standard Conditions)

 $T_{ign} = 632 \text{ °C}$ with air

= 556 $^{\circ}$ C with Oxygen

 $T_t = 2222 \text{ °K}$ (Adiabatic) at $\phi = 1.0$

Lower Combustion limits = 5 %

Theoretical Air/Fuel ratio = 9.52 by Volume

 $S_{\mu} = 0.38 \text{ m/sec}$, at P=1.0 Atmos

From the pollution comparison present on Table (1) appears that the methane fuel has the lowest level, and that will be helpful to reduce the emission quantity.

Table1 Fossil fuel emissions levels (Pound per Billon of Btu energy input, = $1.7876 \times 10^{-3} \text{ kg/Gcal}$)

Pollutant Name	Natural Gas	Oil	Coal
Carbone Dioxide CO ₂	117,000	164,000	208,000
Carbon Monoxide	40	33	208
Nitrogen Oxides	92	448	457
Sulphur Dioxide	1	1,122	2,591
Particulates	7	84	2,744
Mercury	0.000	0.007	0.016

2 Fuel - air mixing technique

In general, the fuel mixed with the oxidant by any of the following technique. These are;

1-Premixed, or 2-Diffuse,

As shown on Fig (2A & 2B), and the burning reaction process for both are similar, but the performance of their heat release will be different. In both the energetic air molecule will strike the fuel ones to initiate the wide reaction and the full combustion phenomena, as shown by three dimensions on Fig (3), which also shows the gases flow pattern [3].

3 Burning Velocity

The burning velocity of any flame can be evaluated from the following fuel-oxidant mixture mass flow rate:



Fig.2. Flame mixing types.



Fig.3. Flame Zones.

Then later when the gas temperature profile known then the gas velocity distribution can be obtained from:

$$S_u = U \times (T_g/T_\infty) \tag{6}$$

4 Computer Program

The flow chart of the present model was computerized in a computer program of flow chart shown on Fig (5). The program was constructed within the MATLAB one, and based on the energy balance of the chain reaction species of the following reaction for methane-air flame:

Fig.5. Flo	w Chart	of the	computer	program
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 $mCH_4 + n(0.210_2 + 0.76N_2) = n_1CO_2 + n_2CO + n_3H_2O + n_4O_2 + n_5H_2 + n_6OH + n_7O + n_8H + n_9N_2 + n_{10}NO$ In present program we used the basic technique of the energy balance followed Ref [2, & 4]. More that all the required data to run the program and calculate the energy terms were obtained from Ref [5, & 6]

5 Results

Then after calculating the energy terms for both the burnt gases and the liberated ones on the Matlab drawing to decide the optimum adiabatic flame temperature. Our computer program the inter-section technique between the heat's lines of the burnt gases and the liberated ones to decide the optimum adiabatic flame temperature as shown on Figs (6 to 9). This program can be used to calculate Adiabatic flame $T_{\rm f.}$



Fig.6. Adiabatic flame temperature decided by using the best fitting curve.



Fig.7. Adiabatic flame temperature decided by using the exact fitting curve.



Fig.8. Species partial pressures at the optimum adiabatic flame temperature.



Fig.9. Effect of the burning pressure on the adiabatic flame temperature.

6 Conclusions

From the present research one will be able to conclude the following points:

1-Such accurate study to any flame can be very helpful to save a significant amount of energy and the fire men to re estimate their extinguishing procedure.

7 Nomenclature

Symbol	Definition	Units
Α	Flame or Flow cross- section area	m ²
A_{f}	Flame surface area	m ²
f	Fuel-Air ratio	unit less
h	Convection coefficient	$W/m^2 \circ C$
m	Methane mole number	mol
m'	Fuel burning mass rate	kg/sec
nior, j	moles number	mol
Р	Pressure	atoms
Q	Heat of reaction	cal/mol
Q_f	Heat losses	W/m ²
r	Radial distant	mm
S _u	Burning velocity	ms ⁻¹
Т	Temperature	°K
U	Gas velocity	ms ⁻¹
Х	Height above burner top	mm
ρ	Gas density	kg/m^3
φ	Fuel– Air mixing ratio	unit less
σ	Stefan Boltzmann law = 5.67×10^{-8}	$W/m^2 \ K^4$
3	Flame or gas emissivity	-
α	Flame or gas absorptivity	-

Notice that air means 0.21O2+ 0.76N2

The following Subscripts are referring to: CH4 Methane gas

- \propto Ambient conditions
- ig Ignition
- f Flame
- *pt* Heat of the burnt gases
- t Heat liberated

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