ANALYSIS OF ALKANE-AIR MIXTURES USING MATLAB/SIMULINK MODEL

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Abstract

The chemical reaction, in which an oxidant reacts with a fuel and results in heat and by products, is called as combustion reaction. One of the most important parameters of combustion process is adiabatic flame temperature which is defined as the maximum temperature achieved by the products during which there is no involvement of both heat and work or the kinetic and potential energy. The significance of calculating adiabatic flame temperature is that it does not only give the idea of thermal stresses induced in the combustion chamber but also controls the amount of pollutants such as carbon oxides and nitrogen oxides released during such reactions. In this paper, first law of thermodynamics is applied to calculate the adiabatic flame temperature of different alkane-air mixtures in steady state condition. A model has been developed for the above analysis in MATLAB/Simulink and variation in adiabatic flame temperature with equivalence ratio has been plotted to study its nature.

Index Terms: Adiabatic flame temperature, Equivalence ratio, MATLAB/SIMULINK

I. INTRODUCTION

The most important technology for providing energy is combustion that has been used by mankind for many years. But it has many environmental problems such as incomplete combustion leads to production of many harmful emissions.

One of the most important properties of combustion reaction is flame temperature. The flame temperature is calculated by applying the energy balance between reactants and products at equilibrium. Flame temperature is the maximum temperature in the reaction zone if the reaction is spatially thin as compared to the rest of the domain of interest [1]. And if there is no heat and work takes place or no change in kinetic and potential energy, then it is referred as adiabatic flame temperature. Adiabatic flame temperature is the maximum temperature that can be achieved by the products during combustion reactions. The significance of calculating the adiabatic flame temperature is that it helps in the prediction of the thermal stresses induced in combustion chamber and controls the harmful gases such as oxides of nitrogen, carbon mono oxide, carbon dioxide etc. that are released during the exhaust process. Thus adiabatic flame temperature helps in designing the combustion chamber and minimization of harmful gases.

A *MATLAB/SIMULINK* model has been developed for this analysis. MATLAB/Simulink, developed by Math Works, is a graphical programming environment for modelling, simulating and analysing multi domain dynamic systems. Its primary interface is a graphical block diagramming tool and a customizable set of block libraries [2]. It offers tight integration with the rest of the MATLAB environment. Applications include creating or designing a model, simulating the model, analysing its results and also testing in real life conditions.

II. THEORETICAL BACKGROUND

In combustion process, the maximum temperature of products can be achieved for the given reactants only when there is no

involvement of work, heat or changes in kinetic or potential energy. This maximum temperature is known as adiabatic flame temperature [3].

Assumptions considered for this analysis are as follows:

- All gases are ideal.
- Steady state reaction.
- No oxidation of N_2.
- No reduction of O_2 and H_2O.
- H_2O and C_8H_{18} are in liquid form and rests are in gaseous form.
- The pressure and temperature of reactants are assumed to be at 0.1MPa and 298 K respectively.

The first law for a steady state, steady flow process can be written in the form.

$$Qc.v. + HR = Wc.v. + HP$$

The above equation can be rewritten as following:

$Qc.v. + \Sigma R\ N_i \times (h_f+\Delta h)_i = Wc.v. + \Sigma P\ N_e \times (h_f+\Delta h)_e$ Since there is no involvement of work and heat,

$$Qc.v. = 0\ \&\ Wc.v. = 0$$

So,

$$\Sigma_R N_i \times (h_f+\Delta h)_i = \Sigma_P N_e \times (h_f+\Delta h)_e \qquad (1)$$

Any combustion reaction can be written as follows: $p(C_mH_n) + q(O_2 + 3.76N_2) \rightarrow a(CO) + b(CO_2) + c(H_2O) + d(N_2)$ Where,

p, q, a, b, c, and d are coefficient of fuel, air, carbon mono oxide, carbon dioxide, water and nitrogen respectively. m and n are the number of carbon and hydrogen atom in the fuel.

$a= (2 \times p \times m) – (2 \times q) + (0.5 \times p \times n)$

$b= (2 \times q) - (0.5 \times p \times n) – (p \times m)$

$c = (0.5 \times p \times n)$

$d = 3.76 \times q$

If a=0, q will give the minimum air required for complete combustion, i.e. $q = (p \times m) + (0.25 \times p \times n)$

From (1),

$\Sigma_R N_i \times (h_f+\Delta h)_i = (h_f \times N_{fuel})$

$\Sigma_P N_e \times (h_f+\Delta h)_e = [\ N_{(CO)} \times (-110541 + \Delta h_{CO,\ T}) + N_{(CO2)} \times (-393456 + \Delta hCO2,\ T) + N(H2O) \times (-241845 + \Delta hH2O,\ T) + N(O2) \times \Delta hO2,\ T + N(N2) \times \Delta hN2,\ T]$

where Δh is a function of temperature.

III. SIMULINK ANALYSIS

For the analysis we have used MATLAB/Simulink, where different blocks are used for different operations. To approach the problem, a simple flow chart has been created which is shown by Fig.1. The relation derived from the first law of thermodynamics is fed into the model using different blocks and operators and analysis is carried out.
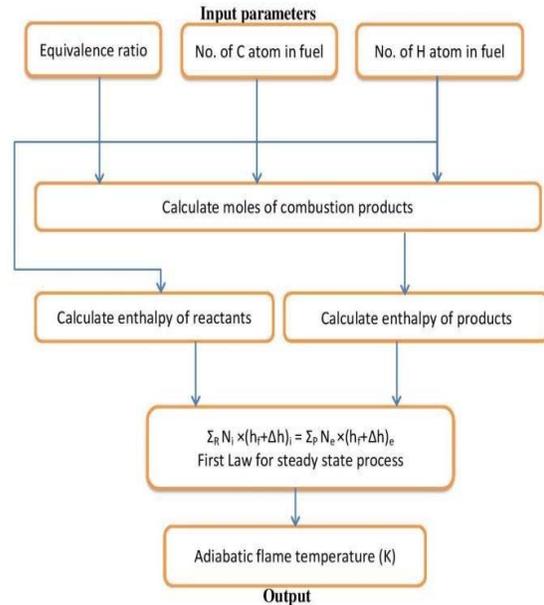

Fig.1: Flow chart

The key feature of the model developed in MATLAB/Simulink is that after feeding different constant properties in 1-D lookup table e.g. enthalpy of fuel, enthalpy of carbon dioxide and water [4] etc. of various alkanes, one may calculate the adiabatic flame temperature for different fuel for different air fuel mixture i.e. for lean, stoichiometric and rich mixture.

IV. RESULTS AND DISCUSSION

Adiabatic flame temperature is one of the most important parameter while designing the combustion chamber. It not only controls thermal stresses induced in the combustion chamber but also minimize the emission of harmful gases. In this work, the effect of equivalence ratio on adiabatic flame temperature is analyzed for different fuel and a graph is plotted between the adiabatic flame temperature and equivalence ratio.
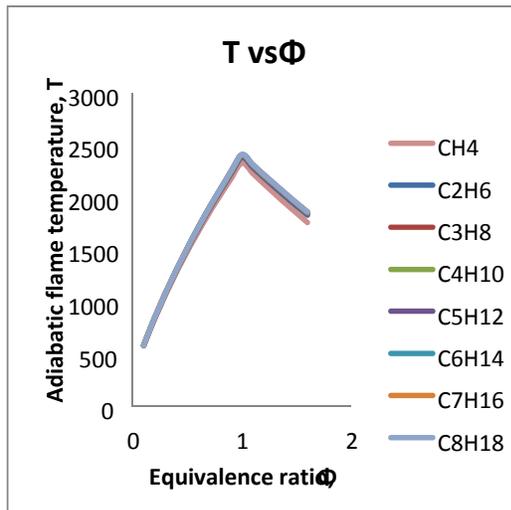
Fig2: Variation of Adiabatic flame temperature with Equivalence ratio

Fig.2 shows the variation adiabatic flame temperature with equivalence ratio from methane (CH_4) to n-octane (C_8H_{18}). By varying equivalence ratio from 0.1 to 1.6, the adiabatic flame temperature first increases and reaches a maxima at $\Phi = 1$ and then start decreasing. It is also observed that as the fuel changes from methane to n-octane, there is a rise in adiabatic flame temperature i.e. as the number of carbon atom in fuel increase, the adiabatic flame temperature increases. This is due to the fact that the enthalpy of n-octane is more negative than the enthalpy of n-heptane and so on.

V. CONCLUSION

In this paper, variation of equivalence ratio was carried out and the corresponding adiabatic flame temperature was calculated with the help

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of MATLAB/Simulink model. It was concluded that the adiabatic flame temperature is maximum in case of stoichiometric reaction and it will decrease if the mixture is lean or rich. By knowing the adiabatic flame temperature, the thermal stresses induced in the combustion chamber can be calculated and making its design easy. Also in case of lean mixture, the emission of harmful gases released from the exhaust, is reduced and thus has lesser impact on the environment.

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Appendix A:

The Fig.3 and Fig.4 show the air fuel mixture model and temperature analysis block respectively. In the Fig.3, three inputs i.e. equivalence ratio and number of C and H atom present in the fuel, are fed which gives the adiabatic flame temperature of that fuel air ratio after temperature analysis
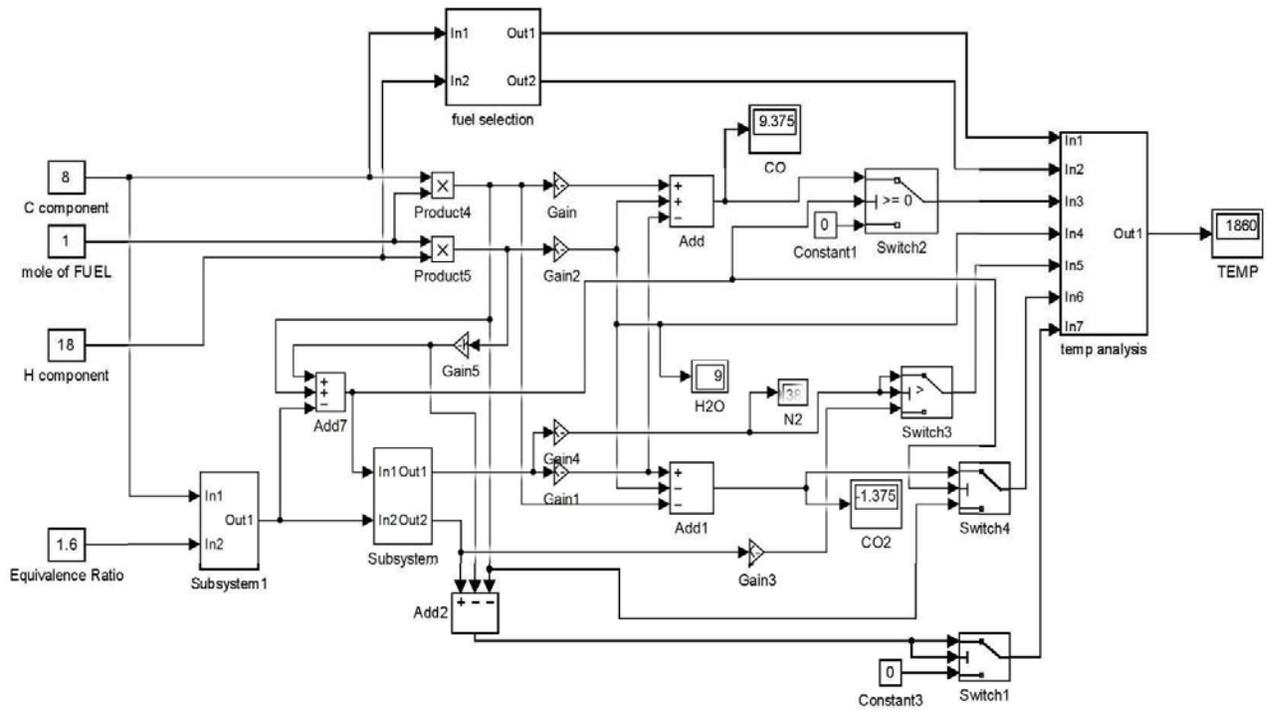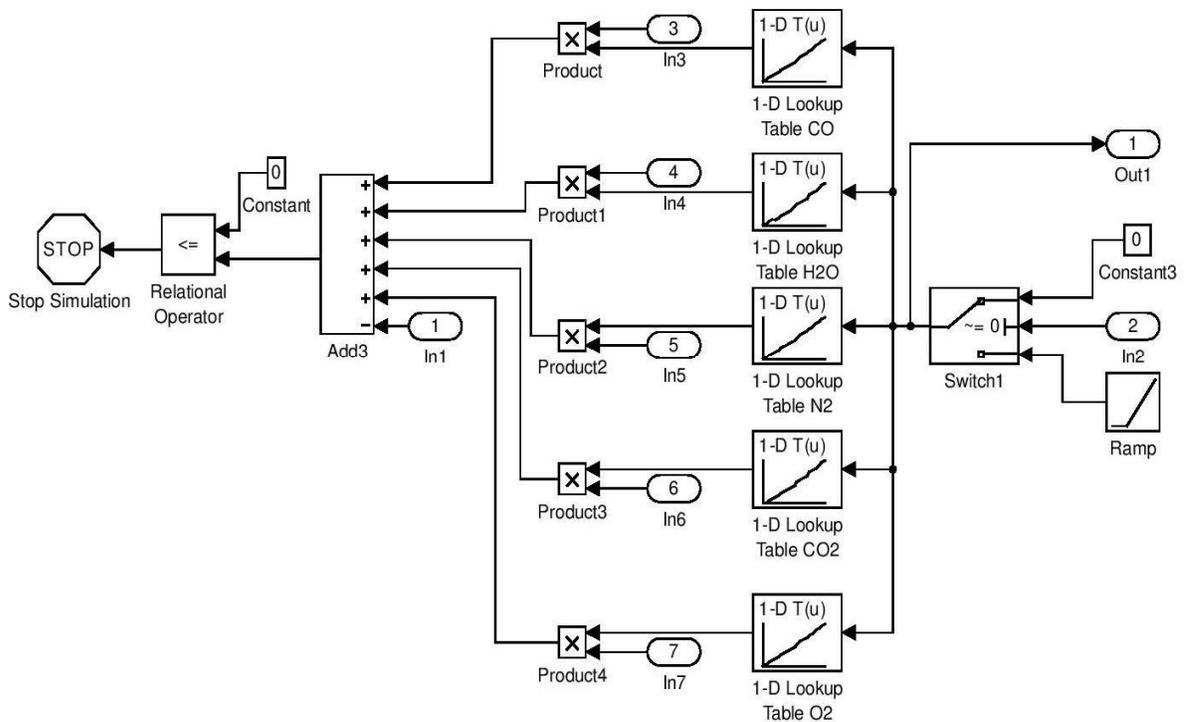
Fig.3 Fuel Air Mixture Block

Fig.4: Temperature Analysis