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A Analysis on Basic Combustion Theory and Issues of Droplets of Liquid Energy Sources

Ashvini Kumar

H.O.D (Mechanical) Sityog institute of Technology Aurangabad Bihar

***Abstract* – Studies have been made of the combustion of droplets of liquid bio fuels such as FAME and the alcohols, especially ethanol and n-butanol, and of pulverised solid biomass materials such as wood and Miscanthus which burn in an analogous fashion. Information is given on the burning rates of both the liquids and the solids and data given on soot formation yields for the different fuels. The mechanism of soot formation is discussed in relation to (1) volatile liquid fuels such as n-heptane, alcohols and aviation fuels, (2) liquid fuels having higher aromatic levels such as diesel fuels, and (3) biomass particle combustion.**

A new theoretical analysis based on heat transfer within the droplet is presented here. It shows that the condensed-phase unsteadiness lasts for about 20-25% of the total burning time. It is concluded that the discrepancies between experimental observations and the predictions of the constant-property quasi-steady analysis cannot be attributed either to gas-phase or condensed-phase unsteadiness.

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INTRODUCTION

For half a century extensive research has been undertaken on the combustion of sprays of conventional fuels for engines and for power generation, and extensive information has been obtained on the rates and mechanism of combustion, on soot and on NOx formation. Generally it is agreed that after the initial stage droplets burn approximately at a rate give by the d2 law even in the case of multi-component fuels such as commercial fuels which have similar physical properties. However in the case of multi-component fuels the sooting propensity is a strong function of the aromatic content even though the burning rates do not vary significantly.

Recently attention has been directed to alternative liquid fuels such as FAME, bio-oil and the alcohols especially bio-ethanol and bio-butanol, only a few measurements have been made previously.

At the same time attention has been directed to the use of finely pulverised biomass materials such as wood and Miscanthus for power station co-firing applications and a number of fundamental studies have been made. Comparison can be made of droplet combustion with the combustion of small solid biomass particles where a large fraction of the cell wall material decomposes to give a gaseous product, and then combustion proceeds in an analogous fashion to the evaporation of a liquid droplet.

Combustion of a single fuel droplet in an oxidising atmosphere has been a subject of investigation over the past two decades. While several reviews have appeared on various aspects of droplet combustion, there are many important features which have yet to be explained. The present paper constitutes a reexamination of the problem of liquid bipropellant droplet combustion and includes analytical studies concerning unsteadiness and variable properties.

The bulk of experimental work reported in the literature is on the combustion of suspended stationary droplets in an oxidising atmosphere - generally air. The porous burner technique has also been in wide use. In the above two techniques the experiments are affected by natural convection; the most striking effect being on the shape of the diffusion flame. The effect is found to be larger in the case of porous spheres of larger diameter. Stationary suspended drops appear to undergo unsteady combustion. The zero-gravity experiments of Japanese workers involve unsteady combustion of free fuel droplets (with no convective influence), but of these three sets of experiments, only the last is relevant to analytical models which invariably assume spherical symmetry.

UNSTEADY CONSEQUENCES IN DROPLET COMBUSTION

The unsteady analysis of Isoda and Kumagai considers only gas phase (g-phase) unsteadiness while neglecting radial convection terms. The solution of the conduction equation invokes the steady-state boundary conditions

$$T = T_f: \quad dT/dr = \dot{m}(H - L)/4\pi r_f^2 \quad \text{at} \quad r = r_f, \tag{1}$$

And

$$T = T_\infty \quad \text{as} \quad r \to \infty. \tag{2}$$

For the above system an analytical solution is possible which is

$$\frac{T - T_\infty}{T_f - T_\infty} = \frac{r_f}{r}\, erfc\left[\frac{r - r_f}{2(\alpha_g t)^{1/2}}\right]. \tag{3}$$

For the conditions (experimental d^2-law) used by Isoda and Kumagai, Eq. (3) with boundary conditions (1) and (2) predicts the SQST solution for d_f/d_s at large times (~1.5 sec). However, the graphical-numerical technique used by the authors shows a significant deviation from the above analytical solution. Another model of g-phase unsteadiness presented in the same report draws heavily from the experimental results and does not constitute a proper check on the theory.

The transient theory of Spalding makes use of a point source at the origin where the fuel is injected into the field to simulate the burning drop. The radial convective velocity is assumed to be zero. By considering only the#-phase unsteadiness, Spalding has shown that the flame initially moves away from and later towards the droplet. The transient analysis as well as the results of Chervinsky constitute a modification of Spalding's work. The study of the above two papers is hampered by the fact that numerical results in the physical plane are not presented.

A recent study on droplet evaporation by Hubbard et al. suggests that the numerical results of Ref. are in error. Hubbard et al. have also shown that gas-phase unsteadiness is insignificant in the evaporation process. The recent report of Waldman on the non-steady combustion of a droplet is based on asymptotic analysis. His results, particularly on the variation of d_f/d_s with time, show discrepancies when compared with experimental results.

SODIUM DROPLET COMBUSTION

Liquid sodium leaked from pipes spreads, scatters in the room. It sometimes forms itself into droplets while falling in atmosphere. These droplets may be ignited and reacted with oxygen with combustion, or may be only solidified into sphere on being cooled. This kind of droplets c|ombustion is sometimes called 'spray combustion\ The droplet behavior depends on the conditions of the atmospheric and the droplet itself. The physical and chemical phenomena around the liquid sodium droplet while falling and combusting in the atmosphere are schematically. Sodium is evaporated from the droplet surface and forms vapor layer. It is transferred by the flow and the diffusion. There are thermal-hydraulic phenomena within and around a liquid sodium droplet, hi the forced convection flow around the droplet, the counter diffusion and reaction occur among the chemical species such as sodium, oxygen and vapor water, and sodium oxide. Sodium and its compounds are condensed and formed into aerosol. It is carried away by the flow and the diffusion.

Chemical species considered in this study are selected based on the experiments about the sodium combustion (Tsai, 1980). Nitrogen (N_2), oxygen (0_2) and vapor steam (H.0) are chosen as atmospheric chemical species. Hydrogen (H_2) is chosen because it is sometimes produced by the sodium-water reaction. Sodium (Na), sodium hydroxide (NaOH), sodium oxide (Na_20) and disodium peroxide (Na_20_2) are chosen as the representative reaction products of the sodium combustion.

EXPERIMENTAL PROCEDURES AND RESULTS

The burning rate experiments consist of photographic examinations of suspended burning droplets and suspended wood particles. These gave information on the decrease in size as a function of time, and hence the burning rates. Relative indications of the amount of soot produced were determined using direct photography and measurements of the soot radiance from the image.

An examination has been made of soot produced which was heated using py-GC-MS temperature programmed analysis. A similar technique has been used for the soot from the wood samples.

Experiments were also undertaken using the porous sphere technique to give information on the mass burning rates and the soot index. A number of fuels were used including pure hydrocarbons, commercial aviation kerosene turbine fuel (Avtur) with an aromatic content of 19.9% and a diesel fuel (D1) with an aromatic content of 29.9%.

SIMULATION OF DROPLET COMBUSTION

In this paper, the combustion of liquid sodium droplet is studied by using the developed computer program, COMET. The burning out of the droplet falling in the air is simulated in this study. The simulation result of the burning rate is compared with the experimental equations of the single droplet combustion of hydrocarbon.

The sphere shape droplet is located in the longitudinal rectangular space. The atmospheric air flows uniformly in the z direction with constant inlet velocity. The number of grid points is 49 x 49 x 97. The grid system is 20mm in width and depth, and

40mm in height. The grid system is hence composed of the cubic volume cells whose length of the side is 0.42mm. The time step size of 0.10ms is selected. The ratio of specific heat of gas is assumed the same as that of ideal gas of 1.40. The mass absorption coefficients (k) of sodium and its compounds are not yet experimentally measured. In this study, the mass absorption coefficient of monochromatic radiation of carbon dioxides (Kondoh, 1977) is used tentatively. The Lennard-Jones potential parameters for all considered chemical species must be given. The parameters of N_2, 0_2, $H_{:}0$ and $H_{:}$ are referenced (Reid, 1985), and those of sodium and its compounds are estimated.

CONCLUSION

The burning rates for oxygenated fuels are quite similar to those for hydrocarbon fuels and the relative rates are capable of being calculated from their physical properties. The burning rates of the volatiles released during the burning of small particles of biomass are also similar to those for hydrocarbons- both being determined by heat transfer considerations.

The rate of the release of the thermal energy is quite different because the calorific values of solid biomass volatiles is lower. A similar feature holds for the bio fuel droplets. The soot forming tendencies vary very significantly depending on the aromatic content of the fuel being considered. For aromatic hydrocarbons, the sooting tendency generally increased with an increase in the number of carbon atoms per molecule. The influence of the fuel-oxygen on sooting behaviour appears to follow the rules set out by Pepiot-Desjardins et al..

The physical phenomena of the sodium droplet combustion are modeled and formulated. Chemical reactions of sodium, oxygen and vapor steam are evaluated by the equation-solving methods of the pressure equilibrium constants. Thermodynamic properties of the mixed gas are evaluated based on the transport theories. Liquid sodium combustion of a single droplet in forced convection flow is numerically simulated in three-dimensional rectangular coordinates. The mechanism of the combustion of the liquid sodium droplet falling in the air was analyzed.

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