Experimental and Numerical Investigation of the Laminar Burning Velocity of Iso-octane – Air Sprays

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1 Introduction

Liquid fuels are widely used in aerospace propulsion and ground transportation systems as well as in stationary power plants. Therefore flame propagation in heterogeneous two-phase systems containing liquid fuel sprays or suspensions in gaseous atmosphere is of fundamental and practical interest. Also, knowledge of flame propagation mechanisms in drop suspensions is important for various industrial safety issues, as in accidental situations large quantities of reactive liquid may be finely dispersed in air. Progress in this field needs to acquire more fundamental knowledge of combustion phenomena in liquid sprays and suspensions. Present work describes investigations undertaken to obtain reliable experimental data and to build a numerical model of flame propagation in drop suspensions in air.

2 Experimental method

Contrary to the case of homogeneous gaseous mixtures, available experimental data on the fundamental parameters of laminar flames (laminar burning velocity, flame thickness, quenching distance, etc.) in two-phase mixtures of liquid sprays dispersed in gaseous atmosphere are rather scarce. One reason comes from the difficulty to generate monodispersed quiescent sprays and disperse them uniformly in closed vessels. As a result, it is difficult to perform experiments in well controlled and reproducible experimental conditions.

We have chosen to study the propagation of laminar flames in tubes of constant cross section. This method is often used in homogeneous gaseous mixtures to determine the laminar burning velocity. Ignition of the gaseous mixture is achieved at the open end of the tube and the flame moves toward the closed end. In this configuration, a quasi-isobaric flame propagates with a constant average spatial speed. The laminar burning velocity can be derived, according to the so-called Gouy method, from measuring the spatial flame speed and determining flame surface. These two parameters can be obtained from cinematographic records of flame propagation.

The experimental setup was purposefully developed. It mainly consisted of a 0.1m x 0.1 m square cross section, 1 m long vertical tube. The tube was made from transparent glass so that it allowed visualization of flame propagation. A schematic of the experimental set up is shown in Fig.1. The liquid spray was generated by means of an ultrasonic atomizer which produced a quasi-monodispersed spray with a near-zero initial velocity. The atomizer was located at the bottom of the setup and suspended liquid drops were transported along the tube by the gas flow to the open upper end. Just before ignition, two pneumatic jacks were actuated and simultaneously closed the upper end of the tube and removed the ultrasonic atomizer from the bottom, which made open the bottom end of the tube. After ignition, the flame propagated toward the top of the tube in quasi-isobaric regime.

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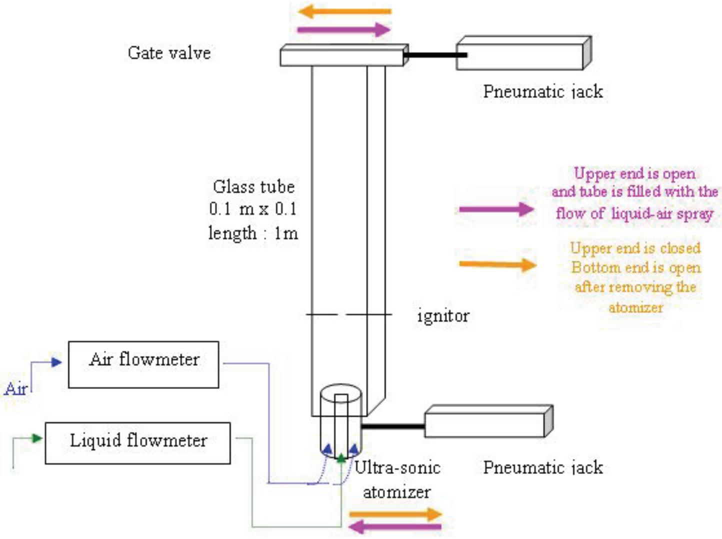

Fig. 1: Schematic of the experimental setup

First, experimental study was conducted for sprays of iso-octane drops in air. Reported here are the results of preliminary experiments. The average diameter of drops was 20 µm. The mixture equivalence ratio φ was estimated to be close to 1.0. A typical sequence of flame propagation is shown in Fig. 2.

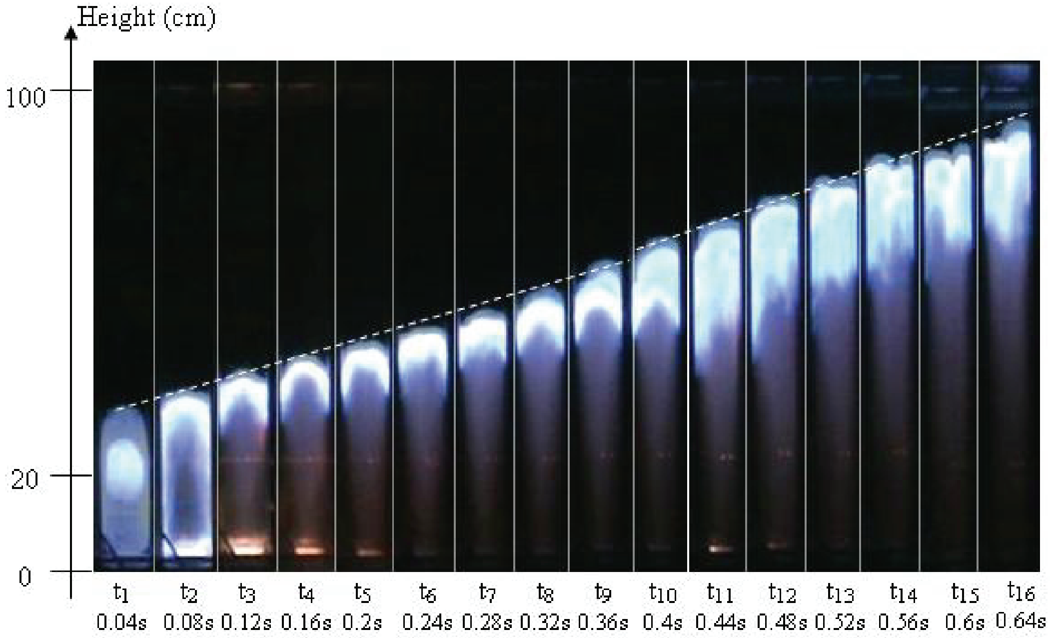

Fig. 2: Sequence of flame propagation in the suspension of *iso*-octane drops in air

After ignition, the flame propagated upward at a quasi constant average velocity. Based on the measured value of the spatial flame front speed and evaluation of flame surface drawn from the analysis of cinematographic records we estimated the laminar burning velocity of the order of magnitude of 28 cm/s. This value is slightly smaller than that of the laminar burning velocity of the gaseous homogeneous mixture of the same composition.

3 Model

There exist several mathematical models of laminar flame propagation in monodispersed drop suspensions [1, 2]. In this paper, a nonempirical model of single drop combustion in a monodisperse spray [3] was coupled with the premixed flame theory to develop a new model of laminar flame propagation in drop suspensions.

The governing equations of the drop combustion model [3] included the partial differential equations of energy conservation in the drop, gas-phase continuity and energy conservation equations, multicomponent diffusion equations for gas-phase species, and the ideal-gas equation of state for the gas phase. All relevant physical properties were considered as functions of pressure and temperature. To ignite a fuel drop, a provision for a thin hot spherical layer of air was made in the initial distribution of gas temperature. The temperature of the hot layer was taken equal to some ignition temperature T_i. The temperature of air outside the hot layer was taken equal to the initial temperature T_0, so that initially the mean gas temperature around the drop $T \approx T_0$. The pressure was taken constant and equal to p_0.

Note that fine fuel drops with the initial diameter of up to 20 μm evaporate faster than ignite in the flame. Therefore only relatively large fuel drops with the initial diameter exceeding 20 μm were considered in this model so far. The drop combustion model makes it possible to determine time histories and spatial distributions of temperature, density, species mass fractions, etc., in the region $r_s \le r \le R$, where r is the radial coordinate, r_s is the drop radius, and R is the "stoichiometric" radius, i.e., the radius of the sphere around a drop containing the amount of air corresponding to the overall equivalence ratio φ in the drop suspension. When the solution for drop combustion is available, it is possible to determine and tabulate the rate of energy release Φ, and the mean values of the rate of variation of the *j*th species in all chemical reactions, w_j, in the region $r_s(t_k) \le r \le R(t_k)$ at any time t_k, as functions of the mean gas temperature T. The functions $\Phi(T)$ and $w_j(T)$ can then be used as the source terms for the equations governing the flame structure in the drop suspension:

$$\frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x}\right) - c\rho_0 u_n \frac{\partial T}{\partial x} + \Phi(T) = 0 \qquad \frac{\partial}{\partial x}\left(\rho D_j \frac{\partial Y_j}{\partial x}\right) - \rho_0 u_n \frac{\partial Y_j}{\partial x} + w_j(T) = 0 \tag{1}$$

where u_n is the laminar flame velocity, ρ is the gas density, c is the gas specific heat, λ is the gas thermal conductivity, and Y_j and D_j are the mass fraction and diffusion coefficient of the *j*th species in the gas phase, respectively. These equations are supplemented with either detailed or overall reaction mechanism of fuel oxidation and the equation of state. Thus, once the functions $\Phi(T)$ and $w_j(T)$ are available from the drop combustion model, one can readily calculate the problem eigenvalue – flame propagation velocity u_n – as well as the spatial distributions of temperature and species mass fractions in the reaction zone, using the standard boundary conditions for Eqs. (1) at $x \to \pm\infty$.

4 Discussion

The combustion model was validated against the experimental data of [4] for laminar flame propagation in the stoichiometric ($\varphi = 1$) *iso*-octane (*iso*-C_8H_{18}) drop suspensions in air at normal atmospheric conditions ($T_0 = 293$ K, $p_0 = 0.1$ MPa). The look-up tables for functions $\Phi(T)$ and $w_j(T)$ were first obtained based on the solution of drop combustion problem for individual *iso*-octane drops of initial diameter $d_{s0} = 2r_{s0} = 60$, 100, and 150 μm with T_i = 1500 K. The overall reaction mechanism of Table 1 was applied, which contains a generalized radical R to take into account water dissociation at elevated temperatures.

Table 1: Overall reaction mechanism of *iso*-octane oxidation

No.	Reaction	h_{ij} kcal/mole	A L, mole, s	m	E kcal/mole
1	C_8H_{18} +8.5O_2 =8CO+9H_2O	696	7.0+14*)	0	50
2	H_2+H_2+O_2 =H_2O+H_2O	114	7.0+13	0	21
3	CO+CO+O_2=CO_2+CO_2	134	8.5+12	0	21
4	CO+H_2O=CO_2+H_2	10	1.0+12	0	41.5
-4	CO_2+H_2 =CO+H_2O	-10	3.1+13	0	49.1
5	H_2O+M=R+R+M	-118	2.8+17	-2	120
-5	R+R+M=H_2O+M	118	9.5+12	-1	0
6	R+H_2+O_2=3R+0.5O_2	118	4.5+14	0	16.4

*) $w_1 = k_1$ [C_8H_{18}][O_2]):

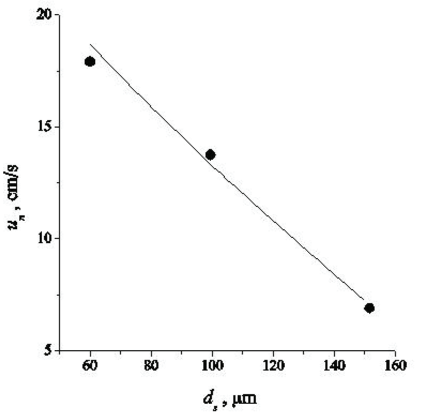

Fig. 3: Comparison of predicted (line) and measured (symbols, [4]) laminar flame velocities in *iso*-octane drop suspensions in air as a function of initial drop diameter. φ =1, T_0 = 293 K, p_0 = 0.1 MPa

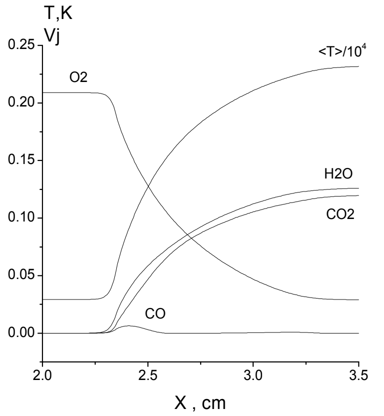

Fig. 4: Predicted spatial distributions of temperature and molar fractions of main species in the laminar flame propagating in *iso*-octane drop suspension in air. d_{s0} = 100 μm . φ =1, T_0 = 293 K, p_0 = 0.1 MPa

As a result of solution of Eqs. (1), the values of u_n and spatial distributions of temperature and species mass fractions were obtained. Figure 3 shows the comparison of predicted and measured values of u_n as a function of d_{s0} . A good qualitative and quantitative agreement between the results is worth mentioning. The predicted value of laminar flame velocity in the gaseous premixed stoichiometric *iso*-octane – air mixture at normal atmospheric conditions is u_n=36 cm/s. It is seen from Fig. 3 that the values of u_n in drop suspensions are considerably lower than in the homogeneous mixture of the same composition. This is evidently caused by smaller (diffusion controlled) mean reaction rates of fuel oxidation in the vicinity of drops. Formally, the trend in Fig. 3 corresponds well with the preliminary measurements of u_n at the experimental setup of Fig. 1 for drops with d_{s0} = 20 μm . Figure 4 shows the predicted spatial distributions of temperature T and molar fractions of main species in the reaction zone of the laminar flame propagating in the suspension of *iso*-octane drops of

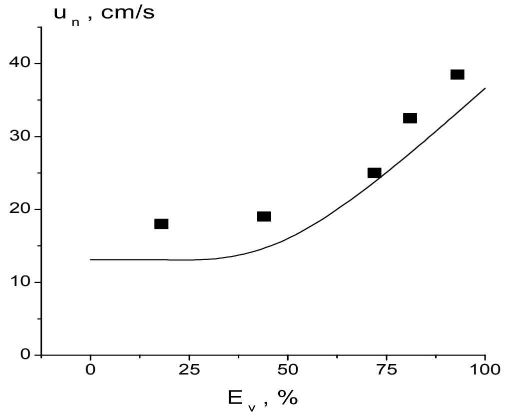

Fig. 5: Predicted (curve) and measured (■ [4]) laminar flame velocities in *iso*-octane drop suspensions in air as a function of the prevaporization degree, E_V. $\varphi = 1$, $T_0 = 293$ K, $p_0 = 0.1$ MPa. At $E_V = 0$, $d_{s0} = 100$ μm

initial diameter $d_{s0} = 100\,\mu$m . The drop suspension flame is about 1 cm thick, which is much thicker than the laminar premixed flame (≈ 0.15 cm). Figure 5 shows the comparison of predicted and measured laminar flame velocities in *iso*-octane drop suspensions depending on the fuel prevaporization degree E_V . Clearly, the partial preliminary vaporization of fuel drops results in the growth of the laminar flame velocity. In the limit E_V = 100%, the suspension flame velocity approaches the value relevant to the premixed laminar flame velocity. A reasonable qualitative and quantitative agreement with the experimental data [4] allows one to treat the model as satisfactory.

4 Conclusions

A new experimental setup for measuring laminar flame propagation velocity in drop sprays has been constructed and preliminary experiments have been made. The reliability of the value derived for the laminar burning velocity depends upon the knowledge of the composition of the two-phase mixture and a correct estimation of the flame surface. First condition is determined by the relaxation of the liquid spray in the conveying air flow. More precise determination of the flame surface needs cinematographic recordings of the flame front from the two sides of the square tube because the flame generally propagates not symmetrically over the cross section and has the tendency to creep preferentially along one wall. These two questions need further investigation in the future. A new model of laminar flame propagation in liquid drop suspensions was developed. The model combined a one-dimensional premixed flame theory and the theory of single drop combustion. Chemical energy release was modeled by the overall reaction mechanism of hydrocarbon oxidation. The model was validated against available experimental data for monodispersed *iso*-octane drop suspensions of different initial size and prevaporization degree. The model can be readily generalized for polydispersed drop suspensions and for turbulent flames.

4 References

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