

Topic: Laminar Flames

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The Influence of Stoichiometric Mixture Fraction on Extinction of Laminar, Nonpremixed DME Flame

Martin Hunyadi-Gall^(a) *Gerald Mairinger*^(a) *Rohit Khare*^(b)

Krithika Narayanaswamy^(b) *Vasudevan Raghavan*^(b)

Kalyanasundaram Seshadri^(a)

^(a)*Department of Mechanical and Aerospace Engineering, University of California at San Diego, La Jolla, California 92093-0411, USA*

^(b)*Department of Mechanical Engineering, Indian Institute of Technology Madras, Chennai, India*
[6pt]

Experimental and computational investigation is carried out to elucidate the influence of stoichiometric mixture fraction on extinction of nonpremixed dimethyl-ether (DME) flames. Measurements are made employing the counterflow configuration. The counterflow burner used in the experimental study has two ducts. From one duct, called the fuel-duct, a fuel stream made up of DME and nitrogen is injected toward the mixing layer. From the other duct, called the oxidizer duct, an oxidizer stream made up of a mixture of oxygen and nitrogen is injected. The mass fraction of the reactants at the boundaries are so chosen that the adiabatic temperature is fixed. The values of the stoichiometric mixture fraction changes from 0.1 to 0.8. The strain rate at extinction is measured as a function of the stoichiometric mixture fraction. With increasing values of the stoichiometric mixture fraction the strain rate at extinction is found to decrease and then increase. Computations are performed with detailed chemistry. The predictions agree with measurements at small values of the stoichiometric mixture fraction, but significant differences are observed at high values of the stoichiometric mixture fraction. Sensitivity analysis was carried out to investigate the reasons for the differences between measurements and computations.

1 Introduction

Conserved scalar quantities, called the mixture fraction, are frequently employed in fundamental studies of the structure of laminar, nonpremixed flames [1–4]. Nonpremixed combustion takes place in mixing layers between a fuel stream that contains the fuel, and an oxidizer stream that contains oxygen. The thin reaction zone of nonpremixed flames will be located at a position where the flux of fuel and the flux of air are in stoichiometric proportions. This location is presumed to be given by the stoichiometric mixture fraction. It has been established from activation-energy asymptotic analysis (AEA) [1–3] and rate-ratio asymptotic analysis (RRA) [4–6] that the flame structure and critical conditions of extinction depend on the stoichiometric mixture fraction and the adiabatic temperature. Here an experimental and computational investigation is carried out to elucidate the influence of stoichiometric mixture fraction on extinction of nonpremixed dimethyl-ether (DME) flames.

2 Formulation

Steady, axisymmetric, laminar flow of two counterflowing streams toward a stagnation plane is considered here. The origin is placed at the stagnation plane, and the spatial coordinate normal to the stagnation plane is x , and the normal component of the flow velocity is represented by u . The stream carrying dimethylether (CH_3OCH_3) mixed with N_2 is called the fuel stream, which is presumed to flow toward the stagnation plane from the region $x < 0$. The stream carrying oxygen (O_2) and nitrogen (N_2) is called the oxidizer stream. It flows toward the stagnation plane from the region $x > 0$. The mass fraction of dimethylether in the fuel stream is $Y_{\text{dme},1}$, and that of O_2 in the oxidizer stream is $Y_{\text{O}_2,2}$. The temperature of the fuel stream is T_1 and that of the oxidizer stream is T_2 .

The diffusivity of any species, i , in comparison to the thermal diffusivity can be characterized by the value of its Lewis number, $Le_i = \lambda/(\rho c_p D_i)$, where D_i the coefficient of diffusion of species i , c_p the heat capacity of the mixture, ρ the density, and λ the coefficient of thermal conductivity. The Lewis number of dimethylether, $Le_{\text{dme}} = 1.5$, while that oxygen and the major products carbon dioxide and water vapor are approximately equal to unity. As a consequence, following the previous analysis of [7, 8], it is convenient to introduce the conserved scalar quantities ξ and ξ_{dme} defined by the equations

$$\begin{aligned} \rho u \frac{d\xi}{dx} - \frac{d}{dx} \left(\frac{\lambda}{c_p} \frac{d\xi}{dx} \right) &= 0 \\ \rho u \frac{d\xi_{\text{dme}}}{dx} - \frac{d}{dx} \left(\frac{\lambda}{c_p Le_{\text{dme}}} \frac{d\xi_{\text{dme}}}{dx} \right) &= 0. \end{aligned} \quad (1)$$

Both ξ and ξ_{dme} are defined to be unity in the fuel stream far from the stagnation plane, and zero in the oxidizer stream far from the stagnation plane. A characteristic diffusion time χ^{-1} deduced from the spatial gradient of ξ is $\chi = 2[\lambda/(\rho c_p)]|\nabla\xi|^2$. The quantity χ represents the scalar dissipation rate. It can be shown that [6–8]

$$2\xi_{\text{dme}} = \text{erfc} \left[\sqrt{Le_{\text{dme}}} \text{erfc}^{-1}(2\xi) \right]. \quad (2)$$

Here erfc^{-1} represents the inverse of the complementary error function and not the reciprocal. It follows from Eq. (2) that

$$d\xi/d\xi_{\text{dme}} = \sqrt{Le_{\text{dme}}} \exp \left\{ (1 - Le_{\text{dme}}) \left[\text{erfc}^{-1}(2\xi) \right]^2 \right\}. \quad (3)$$

For convenience the definitions

$$X_i \equiv Y_i W_{\text{N}_2} / W_i, \quad \tau \equiv c_p W_{\text{N}_2} (T - T_u) / Q_{\text{dme}}, \quad (4)$$

are introduced. Here Y_i and W_i are the mass fraction and molecular weight of species i , W_{N_2} , is the molecular weight of nitrogen, $T_u = 298 \text{ K}$, and Q_{dme} is the heat released per mole of dimethylether consumed in the overall step $\text{CH}_3\text{OCH}_3 + 3\text{O}_2 \rightarrow 2\text{CO}_2 + 3\text{H}_2\text{O}$. At 298 K, $Q_{\text{dme}} = 13,28,000 \text{ J/mol}$, and the adiabatic temperature for chemical reaction described by this

overall step is T_{st}

At the reaction zone, $\xi = \xi_{st}$ and $\xi_{dme} = \xi_{dme,st}$, the mass fractions of CH_3OCH_3 , and O_2 are zero. In the region $\xi > \xi_{st}$ and $\xi_{\text{H}_2} > \xi_{dme,st}$ there is no oxygen, and in the region $\xi < \xi_{st}$ and $\xi_{dme} < \xi_{dme,st}$ there is no fuel. The gradient of τ with respect to ξ , and those of X_i are discontinuous at the reaction zone, $\xi = \xi_{st}$. These gradients in the region $\xi > \xi_{st}$, are represented by the subscript +, and in the region $\xi < \xi_{st}$ by the subscript -. The gradients at ξ_{st+} are

$$\begin{aligned} \frac{1}{Le_{dme}} \frac{dX_{dme}}{d\xi} &= \frac{1}{Le_{dme}} \frac{X_{dme,1}}{1 - \xi_{dme,st}} \frac{d\xi_{dme}}{d\xi} = m \\ \frac{d\tau}{d\xi} &= -\frac{\tau_{st}}{1 - \xi_{st}} = -p \end{aligned} \quad (5)$$

At ξ_{st-} the gradients are

$$\begin{aligned} \frac{dX_{\text{O}_2}}{d\xi} &= -\frac{X_{\text{O}_2,2}}{\xi_{st}} = -c \\ \frac{d\tau}{d\xi} &= \frac{\tau_{st}}{\xi_{st}} = s \end{aligned} \quad (6)$$

Here $\tau_{st} \equiv c_p W_{\text{N}_2} (T_{st} - T_u) / Q_{dme}$. The jump conditions across the reaction zone give $3m = c$, and $\tau_{st} = m\xi_{st} (1 - \xi_{st})$. Hence it follows that

$$\begin{aligned} Y_{dme,1} &= m W_{\text{C}_2\text{H}_6\text{O}} Le_{dme} (1 - \xi_{dme,st}) (d\xi/d\xi_{dme}) / W_{\text{N}_2} \\ Y_{\text{O}_2,2} &= 3m\xi_{st} W_{\text{O}_2} / W_{\text{N}_2} \\ T_{st} &= T_u + m Q_{dme} \xi_{st} (1 - \xi_{st}) / (c_p W_{\text{N}_2}) \end{aligned} \quad (7)$$

3 Experiment and Computation

To characterize the influence of the stoichiometric mixture fraction on critical conditions of extinction, experiments were conducted employing the counterflow configuration. The counterflow burner used in the experimental study has two ducts. From one duct, called the fuel-duct, a fuel stream made up of dimethylether and nitrogen is injected with a speed of V_1 toward the mixing layer. From the other duct, called the oxidizer duct, an oxidizer stream made up of a mixture of oxygen and nitrogen is injected at a speed of V_2 . The experiments are conducted with the initial temperature of the reactants at 298 K. Experimental data on critical conditions of extinction are obtained with the values of $Y_{dme,1}$ and $Y_{\text{O}_2,2}$ so chosen that $T_{st} = 2000$ K. The procedure is as follows, first a value of ξ_{st} is selected. The value of m is calculated from the expression for T_{st} in Eq. (7). This value of m is then used to evaluate the values of $Y_{dme,1}$ and $Y_{\text{O}_2,2}$ from Eq. (7).

A convenient parameter to characterize the residence time is the reciprocal of the strain rate. For the counterflow configuration considered here, the value of the strain rate, defined as the normal gradient of the normal component of the flow velocity, changes from the exit of the fuel duct to the exit of the oxidizer duct [9]. It is discontinuous across the stagnation plane. The local strain rate on the oxidizer side of the stagnation plane, is $a_2 = (2|V_2|/L) \left[1 + |V_1| \sqrt{\rho_1} / (|V_2| \sqrt{\rho_2}) \right]$ [9]. Here, ρ_1 and ρ_2 are the densities of the reactant streams at the injection plane of the fuel duct and at the injection plane of the oxidizer duct, respectively. The separation distance between the ducts is L . The expression for the strain rate is an exact solution of the inviscid equation of motion obtained

in the asymptotic limit of large Reynolds numbers of the reactant streams at the injection planes [9] and are, therefore, fundamentally appropriate representations of the residence time [10].

At a selected ξ_{st} , and calculated values Y_{dme} and $Y_{O_2,2}$ a flame is established at some value of the strain rate less than the extinction strain rate. The strain rate is then increased by increasing V_1 and V_2 simultaneously until extinction is observed. The strain rate at extinction, a_2 is recorded as a function of ξ_{st} .

Numerical computations are performed using FlameMaster [11]). The chemical-kinetic mechanism, and the corresponding thermodynamic and transport properties employed are that of Burke et al [12]. This mechanism is made up of 710 reactions among 113 species. This mechanism has been tested by comparing its predictions with available experimental data obtained using flow reactor, jet-stirred reactor, shock-tube ignition delay times, shock-tube speciation, flame speed, and flame speciation data. Plug-flow boundary conditions are used. At the boundaries of the mixing layer, the mass fluxes of the fuel (and inert) and oxidizer are specified, according to the values used in the experiments. First, a stable flame is established. Then the velocities of the fuel and oxidizer side are increased gradually by increasing their mass fluxes, keeping their momenta same (so that the stagnation plane lies at the center of the computational domain), until the flame extinguishes. Strain rate at this point is recorded as the extinction strain rate.

Figure 1 shows the strain rate at extinction as a function of the stoichiometric mixture fraction, ξ_{st} . The symbols represent experimental data and the lines are predictions. The predictions agree with

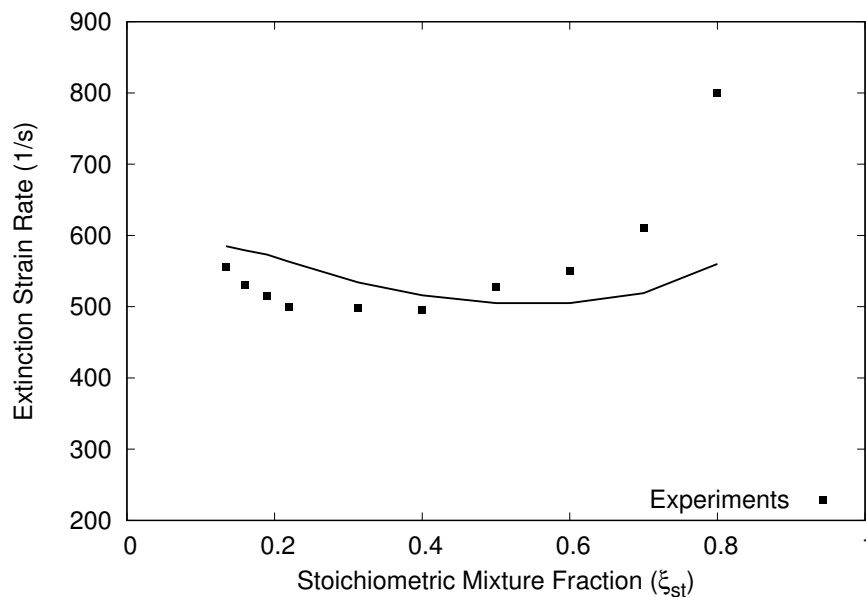


Figure 1: The strain rate at extinction as a function of the stoichiometric mixture fraction, ξ_{st} . The symbols represent experimental data and the lines are predictions.

the measurements at values of ξ_{st} less than 0.5. At higher values of ξ_{st} the predicted values of the extinction strain rate are lower than the measurements.

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References

- [1] N. Peters. *Progress in Energy and Combustion Science*, 10 (1984) 319–339.
- [2] A. Liñán. *Acta Astronautica*, 1 (1974) 1007–1039.
- [3] F. A. Williams. *Combustion Theory*. Addison-Wesley Publishing Company, Redwood City, CA, 2 edition, 1985.
- [4] K. Seshadri. *Proceedings of the Combustion Institute*, 26 (1996) 831–846.
- [5] X. S. Bai and K. Seshadri. *Combustion Theory and Modelling*, 3 (1999) 51–75.
- [6] K. Seshadri and X. S. Bai. *Combustion Science and Technology*, 187 (2015) 3–26.
- [7] K. Seshadri and C. Trevino. *Combustion Science and Technology*, 64 (1989) 243–261.
- [8] U. Niemann, K. Seshadri, and F. A. Williams. *Combustion Theory and Modelling*, 17 (2013) 563–576.
- [9] K. Seshadri and F. A. Williams. *International Journal of Heat and Mass Transfer*, 21 (1978) 251–253.
- [10] H. Schlichting. *Boundary-Layer Theory*. Mc Graw Hill, Inc, 1968.
- [11] H. Pitsch and M. Bollig. Flamemaster, a computer code for homogeneous and one-dimensional laminar flame calculations. Institut für Technische Mechanik, RWTH Aachen.
- [12] U. Burke, K. P. Somers, P. O’Toole, C.M. Zinner, N. Marquet, G. Bourque, E.L. Petersen, W. K. Metcalfe, Z. Serinyel, and H. J. Curran. *Combustion and Flame*, 162 (2015) 315–330.