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# Experimental and computational investigation of partially-premixed methoxymethane flames

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## ABSTRACT

Experimental and computational studies are carried out to elucidate the structure and extinction of laminar partially-premixed flames employing the counterflow configuration. The fuel is methoxymethane (DME). The formulation considers two laminar streams that flow toward a stagnation plane. One stream called the fuel-rich stream is made up of DME ( $\text{CH}_3\text{OCH}_3$ ), and nitrogen ( $\text{N}_2$ ) with small amounts of oxygen ( $\text{O}_2$ ) and the other stream called the fuel-lean stream is made up of  $\text{O}_2$ , and  $\text{N}_2$  with small amounts of  $\text{CH}_3\text{OCH}_3$ . The level of partial premixing is characterized by the equivalence ratio defined as the ratio of the mass of methoxymethane to the mass of oxygen normalized by the corresponding stoichiometric value of this ratio. The equivalence ratio of the fuel-rich stream is  $\phi_r$  and that of the fuel-lean stream is  $\phi_l$ . Previous studies have established that the scalar dissipation rate at extinction depends on the stoichiometric mixture fraction,  $\xi_{st}$ , and the adiabatic flame temperature,  $T_{st}$ . To clarify the chemical influences of partial premixing on extinction, studies are carried at fixed values of  $\xi_{st}$  and  $T_{st}$  and for various values of  $\phi_l$  and  $\phi_r$ . Use of this procedure separates the chemical influences from thermal effects. A previously developed Burke–Schumann (flame-sheet) formulation is employed to estimate the boundary values of the mass fractions of the reactants. Two sets of experiments are conducted, in one set  $\phi_r^{-1} = 0$ , and measurements are made for various selected values of  $\phi_l$ , in the other set  $\phi_l = 0$  and measurements are made for various selected values of  $\phi_r$ . The computations are carried out using the San Diego mechanism that was recently updated to include kinetic steps describing combustion of methoxymethane. For DME addition to the fuel-lean stream, experiments and predictions show that the value of the strain rate at extinction, increases with increasing  $\phi_l$ . For  $\text{O}_2$  addition to the fuel-rich stream, experiments and predictions show very little changes in the values of the strain rate at extinction with increasing  $\phi_r^{-1}$ . The key observation is that addition of DME to the fuel-lean stream enhances the overall reactivity while addition of oxygen to the fuel-rich stream has little influence on the overall reactivity

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## 1. Introduction

There is considerable interest in use of methoxymethane (DME) ( $\text{CH}_3\text{OCH}_3$ ) as fuel for energy conversion in internal combustion engines and gas turbines, because it can be produced at relatively low cost from fossil fuels like coal, and from biomass. DME has a cetane number close to that of Diesel therefore it is suitable for use in compression ignition engines [1,2]. An additional advantage arises from its soot-free combustion in engines as a consequence of the high oxygen content and the absence of C-C bonds, its disadvantage is the low combustion enthalpy as compared to Diesel [3]. Pioneering studies have been carried out by Professor Law and his collaborators on fundamental aspects of premixed

and nonpremixed combustion of DME [4–6] that include ignition and extinction of strained nonpremixed flames [4,6], and structure of coflow flames [5]. These studies have significantly advanced knowledge of influence of low and high temperature chemistry on ignition and extinction and flame structure. In practical systems partially-premixed combustion often takes place. Partially-premixed combustion occurs, for example, if one or both reactant streams of a non-premixed flame are premixed with the other reactant. The structures of highly-diluted [7] and turbulent [8] partially-premixed DME flames have been investigated. Here, an experimental and numerical investigation is carried out to elucidate the influence of premixing of reactants, DME and oxygen ( $\text{O}_2$ ), on structure and critical conditions of extinction. The studies are performed employing the counterflow configuration. The numerical calculations employ detailed chemical-kinetic mechanisms made up of several elementary reactions.

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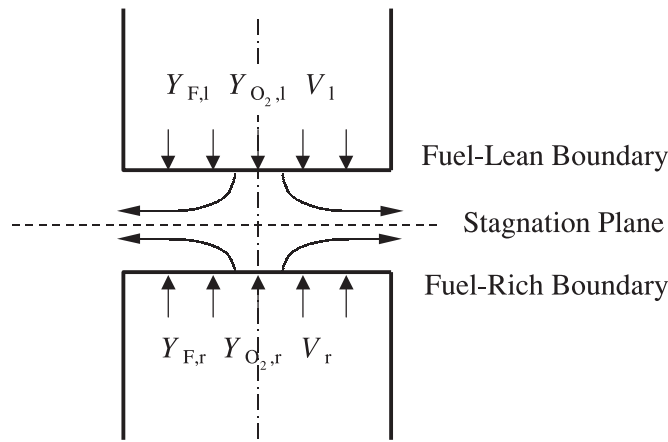


Fig. 1. Schematic illustration of the counterflow configuration.

2. Formulation

A schematic illustration of the counterflow configuration is shown in Fig. 1. Here two counterflowing streams flow toward a stagnation plane. One stream called the fuel-rich stream is injected, at a normal velocity of  $V_r$ , and temperature  $T_r$ , toward the stagnation plane from the fuel-rich boundary. It is primarily made up of  $\text{CH}_3\text{OCH}_3$  (fuel) and  $\text{N}_2$  with small amounts of  $\text{O}_2$ . The other stream, called the fuel-lean stream, is injected, at a normal velocity of  $V_l$ , and temperature  $T_l$ , from the fuel-lean boundary. It is primarily made up of  $\text{O}_2$ , and  $\text{N}_2$  and small amounts of DME. The mass fractions of methoxymethane and oxygen at the fuel-rich boundary are represented by  $Y_{\text{dme},r}$  (or  $Y_{F,r}$ ), and  $Y_{\text{O}_2,r}$ , respectively, and those at the fuel-lean boundary are represented by  $Y_{\text{dme},l}$  (or  $Y_{F,l}$ ), and  $Y_{\text{O}_2,l}$ , respectively. Here  $Y_F$  and  $Y_{\text{O}_2}$  are mass fractions of fuel and oxygen. Subscript r refers to conditions at the fuel-rich boundary, and subscript l refers to conditions at the fuel-lean boundary. The equivalence ratio of the reactant mixture at the fuel-rich boundary is  $\phi_r = Y_{F,r}/(\nu Y_{\text{O}_2,r})$ . The quantity  $\nu = \nu_F W_F/(\nu_{\text{O}_2} W_{\text{O}_2})$ , where  $\nu_F = 1$  and  $\nu_{\text{O}_2} = 3$  are stoichiometric coefficients in the one-step reaction  $\text{CH}_3\text{OCH}_3 + 3 \text{O}_2 \rightarrow 2 \text{CO}_2 + 3 \text{H}_2\text{O}$ , and  $W_F = 0.046 \text{ kg/mol}$  and  $W_{\text{O}_2} = 0.032 \text{ kg/mol}$  are molecular weights of  $\text{CH}_3\text{OCH}_3$  and  $\text{O}_2$ . The equivalence ratio of the reactant mixture at the fuel-lean boundary is  $\phi_l = Y_{F,l}/(\nu Y_{\text{O}_2,l})$ . The flame structure is characterized by  $\phi_r$  and  $\phi_l$ . The present study is carried out for values of  $\phi_r \geq 4.0$  and  $\phi_l \leq 0.3$ . At these conditions previous asymptotic and numerical studies show that multiple reaction zones that are present in the reactive flow-field of a partially premixed flame merge at conditions close to extinction [9–13]. A key objective of this investigation is to compare the critical conditions of extinction when methoxymethane is added to the oxidizer-stream of a nonpremixed flame with those when oxygen is added to the fuel-stream.

In comparing influences of reactant addition to different streams on critical conditions of extinction, choices must be made about what parameters to keep fixed. The structure of the reactive flow-field depends on the four independent boundary values of mass fractions of fuel and oxygen given by  $Y_{\text{dme},r}$ ,  $Y_{\text{dme},l}$ ,  $Y_{\text{O}_2,r}$ , and  $Y_{\text{O}_2,l}$ . In a previous study on partially premixed methane flames, the influence of premixing of the reactants streams on structure and extinction, was carried with the boundary values of the reactants so chosen that the values of the stoichiometric mixture fraction,  $\xi_{\text{st}}$  and adiabatic temperature are fixed,  $T_{\text{st}}$  [14]. These quantities are the flame position in terms of a conserved scalar quantity and the maximum temperature in a Burke–Schumann approximation of the flame structure. This procedure for selecting the

boundary values is employed here. Studies at fixed  $T_{\text{st}}$  highlights the chemical influences of partial premixing by separating them from the thermal effects, and studies at fixed  $\xi_{\text{st}}$  eliminates the physical effects of flame position on extinction [15]. At fixed  $T_{\text{st}}$  and  $\xi_{\text{st}}$  the net flux of the reactants entering the reaction zone are the same irrespective of the direction from which they enter the reaction zone.

To relate the values of  $\xi_{\text{st}}$  and  $T_{\text{st}}$  to the boundary values of the reactants, the approximation that the Lewis number  $Le_i$  for all species, except that of DME, is presumed to be equal to unity. The Lewis number is defined as  $Le_i \equiv \lambda/(\rho c_p D_i)$ , where  $c_p$  is the heat capacity of the mixture,  $\rho$  the density,  $\lambda$  the coefficient of thermal conductivity, and  $D_i$  the coefficient of diffusion of species  $i$ . The Lewis number of DME is represented by  $Le_{\text{dme}} = 1.5$ . Following previous analysis [16–18] two different conserved scalar quantities,  $\xi$ ,  $\xi_{\text{dme}}$  are introduced, defined by the equations

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

Here origin is placed at the stagnation plane, and the spatial coordinate normal to the stagnation plane is the  $x$ , and the normal component of the flow velocity is represented by  $u$ . Both  $\xi$ , and  $\xi_{\text{dme}}$  are defined to be unity in the fuel-rich stream far from the stagnation plane, and zero in the fuel-lean stream far from the stagnation plane. For convenience, the definitions

$$\begin{aligned} X_i &\equiv Y_i W_{\text{N}_2} / W_i, \\ \tau &\equiv c_p W_{\text{N}_2} (T - T_u) / Q_{\text{dme}} \end{aligned} \quad (2)$$

are introduced. Here,  $T_u = T_l + (T_r - T_l)\xi$ , the molecular weight of  $\text{N}_2$  is  $W_{\text{N}_2}$ , and  $Q_{\text{dme}}$  is the heat released per mole of  $\text{CH}_3\text{OCH}_3$  consumed for the overall step  $\text{CH}_3\text{OCH}_3 + 3 \text{O}_2 \rightarrow 2 \text{CO}_2 + 3 \text{H}_2\text{O}$ . For reactants at an temperature of 298 K at the boundaries,  $Q_{\text{dme}} = 13,28,000 \text{ J/mol}$ , and the value of the heat capacity is  $c_p = 1300 \text{ J/(kg} \cdot \text{K)}$ .

In the Burke–Schumann approximation, chemical reactions are presumed to take place in a flamesheet that is located at  $x = x_{\text{st}}$ , the values of  $\xi$  and  $\xi_{\text{dme}}$  at  $x_{\text{st}}$ , are respectively, their stoichiometric values  $\xi_{\text{st}}$  and  $\xi_{\text{dme, st}}$ , and the temperature is  $T_{\text{st}}$ . The profiles of temperature and all species, except that of methoxymethane, are linear function of  $\xi$ , while the profile of  $\text{CH}_3\text{OCH}_3$  is a linear function of  $\xi_{\text{dme}}$ . The gradient of  $\tau$  with respect to  $\xi$ , and those of  $X_i$ , are discontinuous at the reaction zone,  $\xi = \xi_{\text{st}}$ . The gradients in the region  $\xi > \xi_{\text{st}}$  are represented by the subscript + and those in the region  $\xi < \xi_{\text{st}}$  by the subscript -. In view of the stoichiometry of the overall reaction between  $\text{CH}_3\text{OCH}_3$  and  $\text{O}_2$  across the flamesheet the following coupling relation is written

$$\left( \frac{3}{Le_{\text{dme}}} \frac{dX_{\text{dme}}}{d\xi} - \frac{dX_{\text{O}_2}}{d\xi} \right)_+ = \left( \frac{3}{Le_{\text{dme}}} \frac{dX_{\text{dme}}}{d\xi} - \frac{dX_{\text{O}_2}}{d\xi} \right)_-. \quad (3)$$

Energy conservation gives the coupling relation

$$\left( \frac{d\tau}{d\xi} + \frac{1}{Le_{\text{dme}}} \frac{dX_{\text{dme}}}{d\xi} \right)_+ = \left( \frac{d\tau}{d\xi} + \frac{1}{Le_{\text{dme}}} \frac{dX_{\text{dme}}}{d\xi} \right)_-. \quad (4)$$

The gradients at  $\xi_{\text{st}+}$  are

$$\begin{aligned} \frac{1}{Le_{\text{dme}}} \frac{dX_{\text{dme}}}{d\xi} &= \frac{1}{Le_{\text{dme}}} \frac{X_{\text{dme},r}}{1 - \xi_{\text{dme, st}}} \left( \frac{d\xi_{\text{dme}}}{d\xi} \right)_{\xi_{\text{st}}} = m, \\ \frac{dX_{\text{O}_2}}{d\xi} &= \frac{X_{\text{O}_2,r}}{1 - \xi_{\text{st}}} = a, \\ \frac{d\tau}{d\xi} &= -\frac{\tau_{\text{st}}}{1 - \xi_{\text{st}}} = -p. \end{aligned} \quad (5)$$

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