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Rate-ratio asymptotic analysis of the influence of stoichiometric mixture fraction on structure and extinction of laminar, nonpremixed methane flames with comparison to experiments

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Abstract

Activation energy asymptotic analysis and rate-ratio asymptotic analysis of combustion in laminar, nonpremixed flames are often carried out using conserved scalar quantities as independent variables. One such representation of a conserved scalar quantity is the mixture fraction, ξ, based on thermal diffusivity. These analyses are carried out in the asymptotic limit of large Damköhler number, with chemical reactions presumed to take place in a thin reaction zone that is located at $\xi = \xi_{st}$. The quantity ξ_{st} is the stoichiometric mixture fraction. A characteristic diffusion time is given by the reciprocal of the scalar dissipation rate, χ. Previous computational studies have shown that the scalar dissipation rate at extinction depends on ξ_{st} and the maximum flame temperature, T_{st}. Here, a rate-ratio asymptotic analysis is carried out using reduced chemistry to elucidate the influence of ξ_{st} on critical conditions of extinction of methane flames. The scalar dissipation rate at extinction was predicted as a function of ξ_{st} with the mass fractions of reactants so chosen that the adiabatic flame temperature, T_{st}, is fixed. The predictions of the analysis show that with increasing values of ξ_{st}, the scalar dissipation rate at extinction first increases and then decreases. To test the predictions of the asymptotic analysis, critical conditions of extinction are measured on nonpremixed methane flames stabilized in the counterflow configuration. With increasing values of stoichiometric mixture fraction, the strain rate at extinction was found to increase, and the scalar dissipation rate at extinction was found to first increase and then decrease. The predictions of the asymptotic analysis agreed with experiments. A key outcome of the analysis is that with increasing ξ_{st}, the thickness of the regions where oxygen and fuel are

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consumed first increase and the decrease. This is responsible for the observed non-monotonic changes in the values of the scalar dissipation rate at extinction with changes in ξ_{st}.

Keywords: Rate-ratio asymptotic analysis; Conserved scalar; Methane flames; Extinction; Flame structure

1. Introduction

Conserved scalar quantities are frequently employed in fundamental studies of the structure of laminar, nonpremixed flames [1–6]. Nonpremixed combustion takes place in mixing layers between a fuel stream that contains the fuel, and an oxidizer stream that contains oxygen. In analytical studies it is convenient to use these conserved scalar quantities as independent variables. There are many approaches for constructing these variables and they differ in the manner by which the diffusion of the conserved scalar is characterized [7–9]. One such construction is to require the conserved scalar quantity represented by ξ, to satisfy the source-free conservation equation, $\rho(\vec{v}\cdot\vec{\nabla})\xi - \vec{\nabla}\cdot[(\lambda/c_p)\vec{\nabla}\xi] = 0$, where $\vec{v}$ is the velocity vector, ρ the density, λ the thermal conductivity, and c_p the heat capacity per unit mass of the mixture. This equation for ξ is constrained to satisfy the conditions, $\xi = 0$ in the oxidizer stream far from the mixing layer and $\xi = 1$ in the fuel stream [1–6]. A characteristic diffusion is given by the reciprocal of the scalar dissipation rate, $\chi = 2[\lambda/(\rho c_p)]|\vec{\nabla}\xi|^2$, [1–6].

In asymptotic analysis of flame structure, all chemical reactions are presumed to take place in a thin reaction zone, that is located at $\xi = \xi_{st}$. To the leading order, the mass fluxes of fuel and oxygen into the reaction zone are in stoichiometric proportions. On either side of this reaction zone, the chemical reactions are presumed to be frozen [1–5] or the flow-field is inert [6,9–12]. The scalar dissipation rate at $\xi = \xi_{st}$ is represented by χ_{st}. It has been established from activation-energy asymptotic analysis (AEA) [1–5] and rate-ratio asymptotic analysis (RRA) [6,9–12] that the flame structure and critical conditions of extinction depend on ξ_{st} and T_{st}, where T_{st} is the adiabatic flame temperature.

Grudno and Seshadri [13] have carried out a detailed computational study of the influences of ξ_{st} and T_{st} on the strain rate at extinction, a_q, and scalar dissipation rate at extinction, $\chi_{st,q}$, where the subscript q represents conditions at extinction. This study was carried out for $\xi_{st} < 0.5$. The results show that at fixed ξ_{st}, the value of $\chi_{st,q}$ and a_q increase with increasing values of T_{st}. At fixed T_{st}, $\chi_{st,q}$ and a_q also increase with increasing ξ_{st}. Chen and Axelbaum [14] have measured critical conditions of extinction for methane flames at fixed T_{st}, and their results show that the strain rate at extinction increases with increasing ξ_{st}. Song et al. [15] carried out an experimental and computational investigation of the effects of ξ_{st} on propagation speeds of edge flames. They found a close correlation between the influence of ξ_{st} on edge flame propagation speed and the influence of ξ_{st} on critical conditions of extinction of nonpremixed flames. In the present study, a rate-ratio asymptotic analysis is carried out to obtain an improved understanding of the influence of ξ_{st} on flame structure and critical conditions of extinction. Although, the fuel considered here is methane, the results of the analysis can be applied to other hydrocarbon fuels. Critical conditions of extinction are predicted. To test the validity of the analysis experiments are carried out on counterflow methane flame. Critical conditions of extinction are measured at fixed values of T_{st} and various values of ξ_{st}. The predictions of the RRA analysis are compared with the measurements.

2. Rate-ratio asymptotic analysis

Previous rate-ratio asymptotic analyses of methane flames were applied to problems where ξ_{st} was small [9,12]. Here, the analysis is extended to include values of $\xi_{st} > 0.5$. Consider a steady nonpremixed methane flame stabilized in the mixing layer between two laminar streams. One stream, called the fuel stream, is a mixture of methane and nitrogen, and the other stream, called the oxidizer stream, is a mixture of oxygen and nitrogen. In the fuel stream far from the mixing layer, the mass fraction of fuel is represented by $Y_{F,1}$ and the temperature by T_1, and in the oxidizer stream, far from the mixing layer the mass fraction of oxygen is represented by $Y_{O_2,2}$, and the temperature by T_2. Here, subscript F refers to methane, and subscripts 1 and 2, respectively, refer to conditions in the fuel stream and oxidizer stream. If the diffusivity of methane, oxygen, and nitrogen are presumed to be equal to the thermal diffusivity, it has been shown that [9] the stoichiometric mixture fraction, ξ_{st}, is given by

$$\xi_{st} = [1 + 2Y_{F,1}W_{O_2}/(Y_{O_2,2}W_F)]^{-1} \quad (1)$$

and the adiabatic temperature by

$$T_{st} = T_u + Q_F\xi_{st}Y_{F,1}/(W_F c_{p,st}) \quad (2)$$

where W_F and W_{O_2} are the molecular weights of methane and oxygen, $T_u = T_2 + \xi_{st}(T_1 - T_2)$, Q_F is