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Simulations of laminar non-premixed flames of methane with hot combustion products as oxidiser

Jenni A.M. Sidey*, Epaminondas Mastorakos

Hopkinson Laboratory, Department of Engineering, University of Cambridge, Trumpington Street, Cambridge CB2 1PZ, UK

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ABSTRACT

A numerical study has been performed to investigate the behaviour of laminar strained non-premixed flames of CH_4 with hot combustion products as an oxidiser with a focus on various characteristics of MILD combustion. The oxidiser stream was hot combustion products from a $\Phi = 0.6$, 0.7, 0.8, and 0.9 laminar premixed flame, therefore having temperatures above 1650 K and oxygen content, X_{O_2}, below 8%, placing the flames studied in the MILD combustion regime. The simulations used the GRI-Mech 3.0 chemical scheme with a chemiluminescence kinetic sub-mechanism. Heat release rate profiles in MILD flames were spread over a wide region in mixture fraction space. The location of this region and its peak is discussed in comparison to conventional experimental markers for heat release such as the OH* chemiluminescence and pixel-by-pixel product of OH- and CH_2O-PLIF signals. These experimental markers cannot predict the location of peak heat release rate in MILD flames as accurately as in conventional flames due to the extended nature of MILD heat release rate, in contrast to the thin regions of both X_{OH^*} and X_{OH}, presented in both real and mixture fraction space. The effect of strain rate on temperature rise during combustion, ΔT, X_{OH^*}, X_{OH}, and heat release rate is discussed with an analysis of extinction behaviour. MILD flames produced NO through both thermal and prompt NO mechanisms, with both the high temperatures and initial NO concentrations in the oxidiser significantly affecting reaction rate behaviour. The simulations provide insights to some experimental observations usually associated with MILD combustion.

1. Introduction

The study of autoignition, stabilisation, and extinction are essential to the understanding of combustion processes in practical systems employing non-premixed flames. In particular, the study of laminar counterflow flames [1] allows for the investigation of the effect of strain and composition on key flame characteristics. The usefulness of the counterflow flame may be extended to combustion problems with unconventional and more complex chemistries, including those involving the heavily preheated and diluted, or moderate or intense low oxygen dilution (MILD), combustion. The MILD combustion regime, defined by Cavaliere and de Joannon [2], includes processes in which reactants are preheated above a temperature at which they will autoignite and diluted such that the rise in temperature during combustion is low. These processes have been studied in various fundamental and applied devices, often in counter or cross flowing configurations [3–8].

Mastorakos et al. [9] studied the effect of simultaneous preheat and dilution on turbulent counterflow flames experimentally by flowing premixed fuel and air against hot combustion products from a second premixed flame. They reported that, even at very high strain rates, MILD flames would not extinguish, a finding consistent with theoretical work [10]. The absence of an extinction strain rate under heavily diluted and preheated conditions was also observed by Choi and Katsuki [11] along with a reduction in NO emission from counterflowing fuel and low-oxygen oxidiser mixed with an inert gas, a conclusion reported again in later work [12]. Diluted and preheated chemistry details were discussed by de Joannon et al. [8,13,14], including the wider region of heat release rate (HRR) associated with MILD flames and the lack of correlation between the location of the stoichiometric mixture fraction, ξ_{st}, and peak HRR in mixture fraction space. De Joannon et al. also reported a smooth transition to a non-burning solution [13,15], a finding synonymous with the non-extinguishing characteristic reported previously [9–11]. Further discussions surrounding extended HRR and reduced NO formation were presented by Abtahizadeh et al. [16] who reported that the autoignition delay time, τ_{ign}, of various fuel and oxidiser stream configurations decreases with increasing dilution, a result consistent with a recent numerical study [17]. Coriton et al. [18,19] investigated the effect

* Corresponding author.
E-mail address: jams4@cam.ac.uk (J.A.M. Sidey).

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of hot product stoichiometry and flame heat loss on laminar counterflow flames, concluding that, in agreement with the work discussed here, a mode without sudden extinction behaviour occurs when sufficient oxidising species are present in the hot combustion product stream. They identified the role of key radical pools in sudden versus smooth extinction behaviour and concluded that the thickening of the heat release rate profile under MILD conditions was due to a shift in OH and O production rates [18].

With few exceptions [18,20], numerical studies that may be considered relevant to MILD combustion have been primarily concerned with understanding the effects of inert dilution rather than dilution with equilibrium hot combustion products containing radical species near the adiabatic flame temperature, as would occur in most practical systems. Studies investigating autoignition delay time [17,21] and counterflow flames [8] reported that MILD combustion behaviour is sensitive to diluent nature as ignition characteristics are significantly affected by the presence of radial hot product species. Further, since preheat and dilution have been shown to alter non-premixed heat release characteristics [13,14,16], it is essential to investigate the effect of hot product dilution on heat release rate profiles and experimental markers used to map them. In particular, the experimental technique of using the pixel-by-pixel product of OH- and CH_2O-PLIF signals is conventionally used as a marker of heat release for both gaseous [22–24] and, more recently, liquid fuels [25]. Although MILD flames have been studied experimentally using optical imaging techniques such in a variety of premixed [26] and non-premixed [27–30] fundamental configurations, the applicability of this technique to MILD combustion systems would be particularly useful considering the regime's unusual heat release behaviour.

This work is aimed at investigating the fundamental properties of heavily preheated and diluted flames at varying rates of strain with a focus on a better understanding of flame structure and experimentally relevant quantities as markers of HRR. These quantities are of interest not only for their informative nature, but for the relative ease of their measurement with well established optical diagnostic techniques.

It is worthwhile to note that this work has been developed as a fundamental examination of the properties of fuel counterflowing with hot combustion products of varying composition at various strain rates. In practical systems, heat loss effects will lower the temperature of the hot combustion products while dilution itself will be less extensive. Nevertheless, the present paper studies a canonical combustion problem that offers insights for practical systems utilising hot product dilution or recirculation.

The results presented in this paper will be introduced with a discussion on the changes in counterflow flame structure arising from simultaneous preheat and dilution with a focus on intermediate species and NO production. Mole fraction of OH, X_{OH}, CH_2O, X_{CH_2O}, and the excited emission of OH, X_{OH^*}, for MILD and conventional flames is discussed in relation to HRR, CH_4 consumption rate, $\dot{\omega}_{CH_4}$, temperature rise, δT and strain rate, A. This structure, as well as the extension of the extinction limits which comes with extensive preheat and dilution, is discussed in relation to conventional non-premixed flames.

2. Method

A laminar counterflow non-premixed flame (Fig. 1) of cold CH_4 with an oxidiser of either cold air or hot combustion products from a premixed flame is considered. This configuration is described by the species mass fraction and temperature balance equations in mixture fraction, ξ, space, according to the definition described by Bilger et al. [31] by Eqs. (1) and (2) respectively [32].

$$\rho\frac{\partial Y_k}{\partial t} = \dot{\omega}_k + \rho N\frac{\partial^2 Y_k}{\partial \xi^2} \tag{1}$$

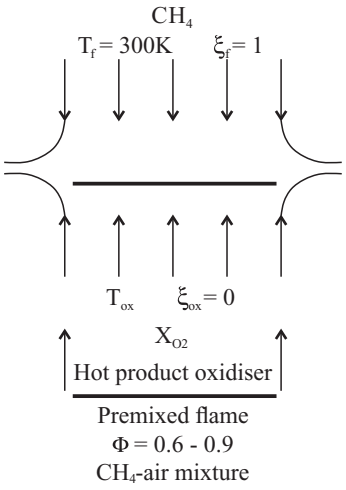

Fig. 1. Laminar counterflow diffusion flame schematic.

Table 1
Oxidiser stream conditions.

Case	T (K)	X_{O_2}	X_{H_2O}	X_{CO}	X_{OH}	X_{NO}	ξ_{st}
Air	298	0.21	0	0	0	0	0.055
0.6	1657	0.08	0.12	0.06	2.2×10^{-4}	2.2×10^{-6}	0.011
0.7	1838	0.06	0.14	0.07	7.3×10^{-4}	1.2×10^{-5}	0.008
0.8	1996	0.04	0.15	0.08	1.6×10^{-3}	9.7×10^{-5}	0.006
0.9	2133	0.02	0.17	0.08	2.7×10^{-3}	5.0×10^{-4}	0.003

$$\rho\frac{\partial T}{\partial t} = \dot{\omega}_T + \rho N\frac{\partial^2 T}{\partial \xi^2} \tag{2}$$

Along with the cold air oxidiser case, four hot product cases were considered: hot products from a 0.6, 0.7, 0.8, and 0.9 premixed flame. With these hot combustion products as an oxidiser, diluted cases reported here correspond to the "hot oxidiser diluted oxidiser" (HODO) sub-category of preheated and diluted combustion defined in Ref. [33]. The hot combustion products were calculated with a laminar freely propagating premixed flame code and allowed to equilibrate in a plug flow reactor. The temperature, T_{ox}, and molar concentrations, X_i, of the counterflow oxidisers, including cold air and hot products, are listed in Table 1. This configuration mimics adiabatic recirculation combustion systems where hot combustion products with coupled composition and temperature characteristics are burned with fresh, cold fuel.

Simulations were performed with COSILAB [34] and the GRI-Mech 3.0 chemical mechanism [35] supplemented with chemiluminescent species [36]. The expanded mechanism, evaluated in comparison with premixed and non-premixed methane-air flames [36], utilises excited species OH* and CH* rate constants from Carl et al. [37] and Elsamra et al. [38] and collisional quenching data from Tamura et al. [39]. The mechanism was developed and assessed through a comparison of the predicted OH* and HCO mole fraction profiles, the product of the OH and CH_2O mole fraction profiles, and the heat release rate over a range of non-premixed CH_4–air compositions and strain rates. It was found that the OH* mole fraction region was capable of marking the peak HRR region as well as the product of the OH and CH_2O regions in conventional flames [36]. This validation is especially useful considering the context of this work as an analysis of the ability of the OH* mechanism to mark a MILD flame HRR region experimentally. This will be discussed in detail in the results section of this paper.

All simulations were performed at atmospheric pressure with mixture averaged transport properties. The steady time step size was chosen to be 1×10^{-6} s while the relative and absolute tolerances were 1×10^{-5} and 1×10^{-9} respectively.

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