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OPPOSED JET FLAMES OF LEAN PREMIXED METHANE-AIR REACTANTS VS. HOT PRODUCTS

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ABSTRACT

To understand the interaction between hot products and lean limit reactant mixture distributions, two opposed jet flames of lean premixed CH₄-air (either $\phi=0.63$ or $\phi=0.50$) versus hot products are studied in an optically accessible burner and compared to numerical simulations. A lean H₂-air ($\phi=0.4$) flame generates the hot products so that their effect on the formation of CO₂ can be seen. A previous investigation of a C₃H₈-fueled flame under very lean conditions showed large discrepancies in the measured and predicted CO₂ profiles, indicating further investigation is needed for lean hydrocarbon combustion. A CH₄-fueled flame is a good alternative to a C₃H₈ flame because of CH₄'s better-understood chemical kinetics and an available validated mechanism (GRI-Mech 3.0). A visible Raman system is used for major species concentration measurements and is equipped with a new optical collection system that gives better discrimination against flame background emission. An opposed jet burner is used that has been improved with a new porous metal plate mounted flush to the exit so that the H₂-air flame is uniform across the nozzle diameter. Experimental results show very good agreement with numerical simulation for profiles of concentration and temperature and demonstrate reliability of the CH₄ mechanism for these very lean opposed jet flames of CH₄-air versus hot products.

INTRODUCTION

Lean direct injection of fuel in combustion devices promises improved fuel economy in spark ignition engines. It has the advantages of low fuel consumption and high power output [1]. In traditional spark ignition engines, homogeneously premixed reactions occur near

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the stoichiometric condition. However, in lean direct injection systems, the fuel is directly injected into the combustor without premixing under overall lean conditions stratifying the fuel into lean and rich regions. This stratification improves fuel economy in both part load and full load conditions. In part load operation, reduction of pumping work (throttle loss) is the principal contribution to fuel economy. Also contributing, but to a smaller degree, is the reduction of wall heat loss and exhaust energy [2]. For full load operation, fuel charge cooling leads to lower temperatures in the cylinder and allows a higher compression ratio, contributing to improved fuel economy. During burning, lean- and rich-limit reactants are supported by mixing with hot products.

Direct injection of the fuel into the center of the cylinder late in the compression stroke just prior to the spark leads to inhomogeneous regions: i.e. the simultaneous formation of stoichiometric, rich, and lean flames inside the cylinder. As shown in Fig. 1, the fuel spray can impinge on the cylinder head to form the various regions. However, lean direct injection of hydrocarbon fuel may cause excess pollutant formation. Unburned hydrocarbons can be produced in the lean regions where the flame is so lean that the flame is extinguished and the fuel is not completely consumed.

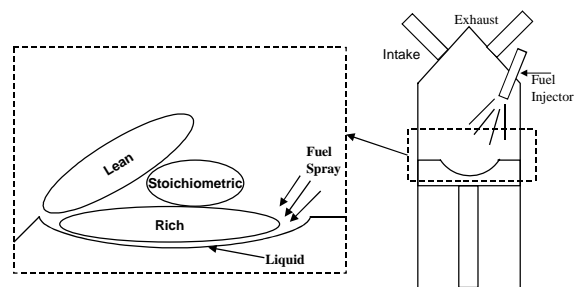


Figure 1. Schematic of stratified charge operation in DISI engine.

The opposed jet burner (shown in Fig. 2) generates ideal counterflow flames that are widely used to study chemical kinetics and species transport

under the influence of aerodynamic stretch. For example, gas sampling, thermocouple probes, and LDV were used to measure the species concentration, flame temperature, and axial velocities for partially premixed counterflow flames [3]. Also, ultraviolet laser-induced Raman scattering was used to study H₂-air diffusion flames from a counterflow burner [4,5] and a partially premixed CH₄-air versus air flame structure was investigated [6].

Previous investigations [7,8] by this group for opposed jet flames of very lean propane-air versus hot products show discrepancies in CO₂ concentration between experimental data and numerical simulation. Since lean-limit combustion phenomena determine emissions of unburnt hydrocarbons in stratified combustion, it is necessary to further investigate lean-limit combustion. Rather than use C₃H₈, CH₄ is used in the present work because of its well-understood chemical kinetics and availability of a well-validated mechanism (GRI-Mech).

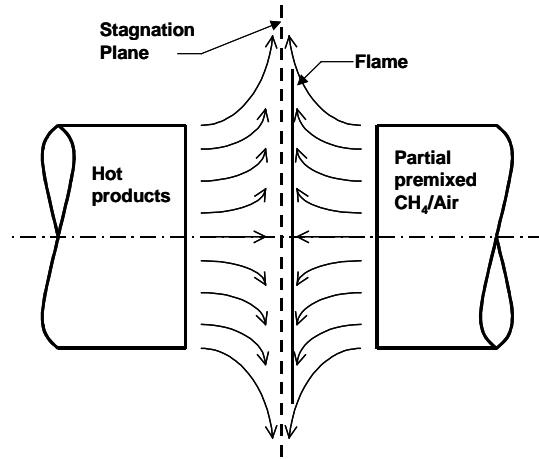


Figure 2. Opposed jet flame schematic: hot products vs. lean reactants

EXPERIMENTS

Measurements of major species and temperature are made along the centerline of an opposed jet burner. A schematic of the visible Raman system is shown in Fig. 3. A 532 nm Nd:YAG laser beam is stretched in time with a beam splitter and focused by a 0.3 m lens. A Stanford Research Systems DG535 pulse generator synchronizes the trigger signals in the system. The Raman light collecting system

in [7,8] is modified by replacing the F/1.5 Cassegrain with a 75 mm diameter F/2 lens. The collimated light from this F/2 lens is focused by a 75 mm diameter F/7.5 lens, passed through a ferroelectric shutter, a mechanical shutter, and an entrance slit to the 0.65 m spectrometer (SPEX 1800, 0.75-meter Czerny Turner Spectrometer, modified to 0.65 m). A mechanical shutter (Uniblitz) is used as an external shutter for the liquid nitrogen cooled CCD camera but has a

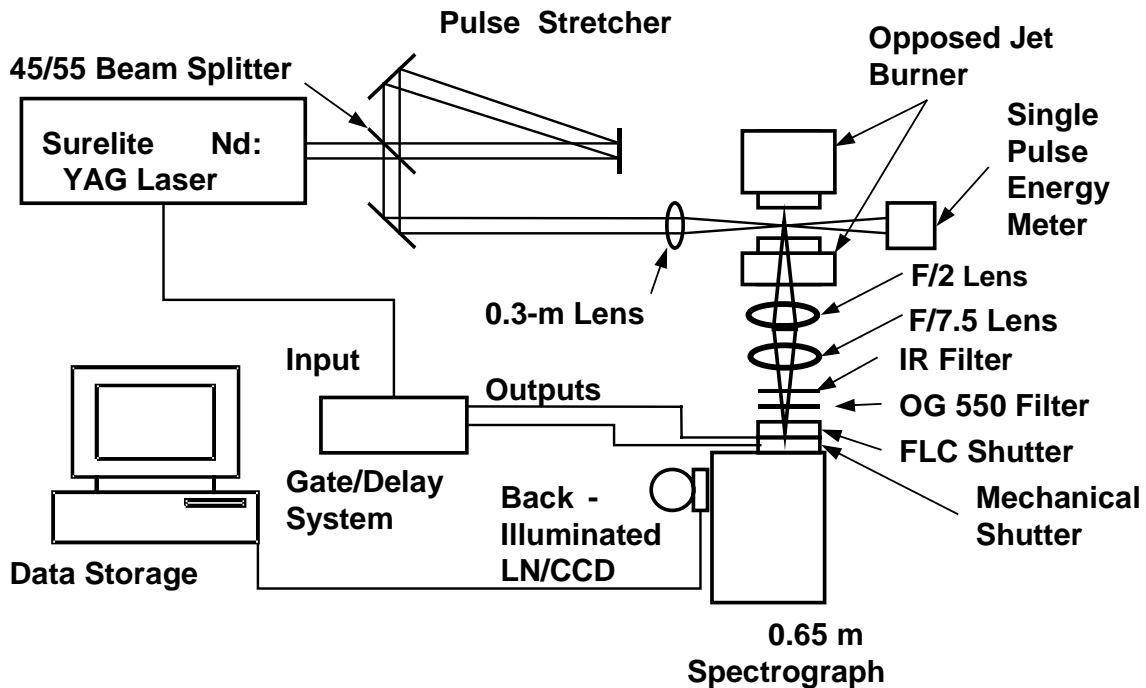


Figure 3. Laser system schematic

relatively long exposure time (6 ms). A ferroelectric liquid crystal shutter is placed in front of the mechanical shutter to cut off flame luminosity into the spectrometer by its short exposure time (30 μ s). An orange Schott glass filter is placed in front of the entrance slit to block any stray 532 nm light. A separate long pass filter (750 nm cutoff) is mounted at the entrance slit to eliminate the infrared radiation from the flame.

A liquid-nitrogen-cooled, charge-coupled-device (LN/CCD) is used to obtain Raman spectra. The LN/CCD camera has a 1024 x 1024 pixel chip, mounted to the back plane of the spectrometer. The chip is back-illuminated to give high quantum efficiency in the visible. The measuring sample volume is a cylinder (length is 4.7 mm and diameter is 0.2 mm). For the planar flame measurement, the 0.2 mm dimension is transverse to the concentration gradient. Thus, the 0.2 mm dimension is the spatial resolution of the system. The sample volume length is limited by the entrance slit image and is about 4.7 mm. The planar flame composition doesn't vary along the 4.7 mm beam length and hence the 1024 pixels along the spatial dimensions are binned into one super pixel.

The opposed jet burner used for this work was modified from the design by Seshadri [4] and was described in detail in reference [7]. It consists of two 25 mm diameter straight jets, which are separated by 12.5 mm. The nozzle exits are further modified for this work. For the top jet nozzle exit, there are two pieces of fine (100#) mesh screen and steel wool to keep the flow uniform. The last mesh screen is mounted by a retaining ring and it is 3 mm away from the nozzle exit. The experimental data are obtained along centerline, so the actual distance between two jets includes this extra 3 mm length and it is 15.5 mm. For the bottom jet nozzle exit, a sintered metal plate (20 μ m particle size) is mounted flush to the exit plane instead of mesh screens because it produces a H₂-air flame that has less tendency to attach to the burner than for the situations where screens are used as in Refs. 7 and 8. Glass beads (6 mm diameter) are also used in the bottom jet under the sintered metal plate. If the momenta of the two flows are balanced, a stagnation plane exists halfway between the two jets. For the bottom jet, co-flow nitrogen shields the flame and prevents outside air from mixing with the jet. The hot exhaust gas is sucked into an annular exhaust section around the top jet. The top jet and annular exhaust are cooled by a jacket water system.

FLAMES EXAMINED

Pollutants can be formed in very lean regions of direct injection engines, but the presence of hot products can improve combustion in these regions. In this work we study how hot products support very lean combustion by using an opposed jet flame as a model. Detailed comparisons between experimental data and numerical simulation were made for an opposed C₃H₈-air flame

versus hot products in a previous study [7,8]. As mentioned earlier, CH₄ fuel is a good alternate to C₃H₈ because of CH₄'s well-known kinetics. Two opposed jet flames are selected to simulate the following lean combustion situations: $\phi=0.63$ and $\phi=0.50$ premixed CH₄-air mixtures. Each of them has a jet of lean H₂-air premixed reactants ($\phi=0.4$) impinging upon a jet of premixed CH₄-air reactants. Since H₂O and CO₂ are the major products of a stoichiometric hydrocarbon reaction, it is convenient to form hot products from a lean H₂-air ($\phi=0.4$) premixed flame. This choice is based on the fact that the premixed H₂ flame has a fast laminar flame speed relative to the premixed hydrocarbon-air flame. Therefore the effect of strain rate on CH₄ flames can be studied individually, without considering the influence of strain rate on H₂-air flames. Another advantage is that no carbon exists in the H₂-air flame products and thus, all the carbon-bearing products (i.e., CO₂ or CO) come from the hydrocarbon-air premixed flames. Thus one can easily see if the hot products lead to the additional burning of the hydrocarbon fuel. An issue with lean H₂-air mixtures is the difficulty to obtain a lifted premixed H₂ flame due to its high laminar flame velocity. With the use of sintered metal, the H₂-air flame, though not completely detached, is at least partially detached.

The axial strain rate a of counterflow flames is given by Kim et al. [9]:

$$a = \frac{2V_O}{L} \left(1 + \frac{V_F \sqrt{\rho_F}}{V_O \sqrt{\rho_O}} \right)$$

where V is the jet exit velocity, ρ is the gas density, L is the jet separation and subscripts F and O denote the two jets, respectively. The counterflow flame at high flow rates can cross the stagnation plane into the hot products side to form a so-called "negative flame speed" flame [10]. The definition of "negative flame speed" stemmed from the original definition of laminar flame velocity that is opposite of the convective velocity at the front edge of the preheat zone of a planar one-dimensional flame. Normally, the bulk convective motion directs the fresh unburned mixture through the flame zone to form burned products.

UNCERTAINTY

Based on photon shot noise calculations, typical uncertainties for the species mole fraction and temperature measurement are listed in Table 1. The uncertainties are functions of both the net

wavelength-integrated Raman signal strength and the amount of background interference that must be subtracted to obtain a net Raman signal. Background interference is due to both continuous flame luminosity (corrected by subtracting an image obtained with the laser off from the Raman image obtained with the laser on) and laser-induced background (corrected by subtracting an interference amount determined by the laser-induced background on both sides of a Raman signal). Uncertainties for flame temperature measurements are below or close 1%. Uncertainties for major species mole fraction are below 6%, except for the very small CO₂ mole fraction measurement in the very lean negative flame speed flame. Uncertainty for minor species CO is up to 38% for methane-air ($\phi=0.63$) flame and it is not available (not detectable) for very lean negative flame speed flame ($\phi=0.50$). These uncertainties are just based on shot noise statistics and other uncertainties such as systematic errors in the calibration process, can also be important.

Table 1. Uncertainties for mole fraction and temperature

ϕ	CO ₂	O ₂	CO	N ₂	CH ₄	H ₂ O	T
0.63	6%	2%	38%	<1%	5%	2%	1%
0.50	32%	2%	N/A	<1%	4%	1.9%	1%

REACTION MECHANISM

The chemical kinetic mechanism used for this work is GRI-Mech 3.0, which involves 325 elementary reactions and 53 species. The related assessment of reaction mechanisms for counterflow rich methane-air partially premixed flames was given previously [11]. The GRI-Mech 3.0 kinetics gives excellent prediction of the premixed flames speeds, flammability limits and nonpremixed flame structure. Therefore it is used for this work.

RESULTS AND DISCUSSION

(1) Raman Spectral Graphs

Figure 4 shows a set of Raman spectral graphs from the partially premixed opposed jet flame: CH₄-air ($\phi=0.63$) versus H₂-air ($\phi=0.40$). They are four representative spectra for different locations along the centerline of the opposed jet burner. Each spectrum is the result of a 600 shots accumulation of light signals onto the CCD, and each spectrum has background luminosity subtracted. The spectrum at location 3.25 mm represents cold CH₄-air reactants zone; the spectrum at location 4.75 mm represents premixed CH₄-air flame zone; the spectrum at location 11.25 mm represents a lean H₂-air

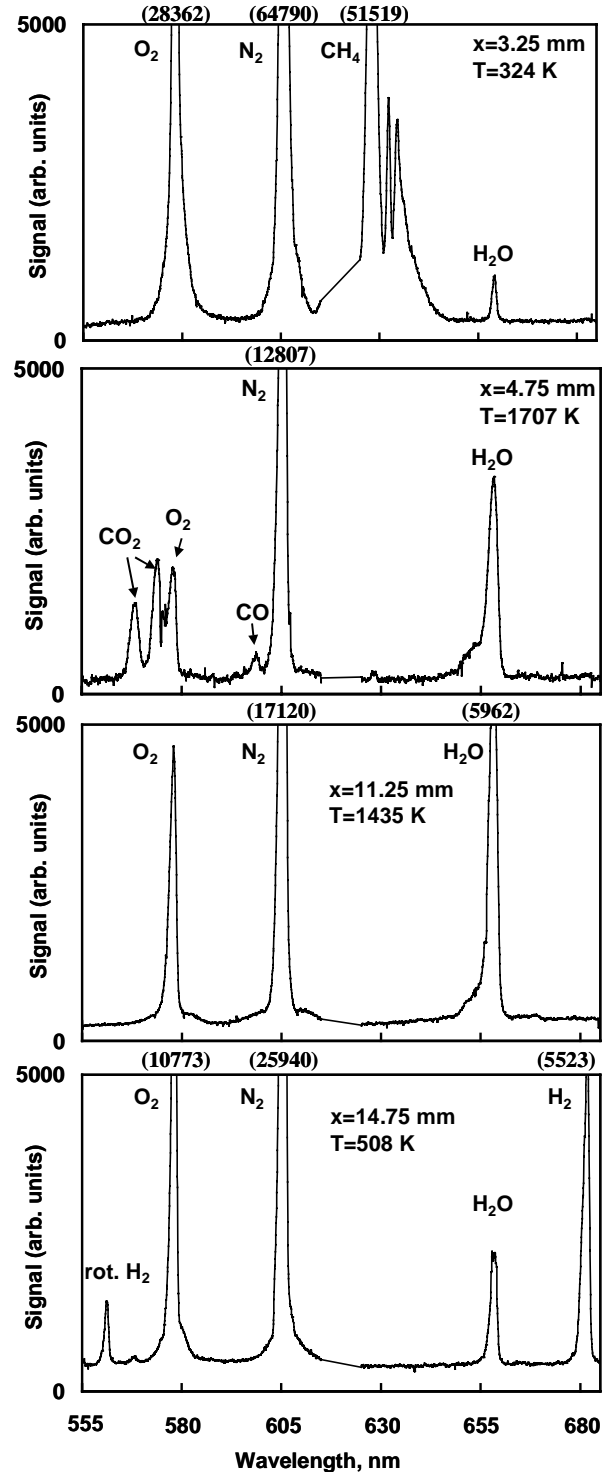


Figure 4. Set of Raman Spectra obtained in partially premixed opposed jet flame: CH₄-air ($\phi=0.63$) versus H₂-air($\phi=0.40$)

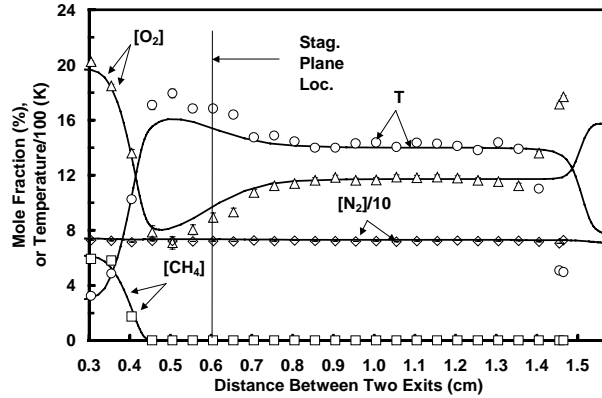


Figure 5. Experimental and numerically-predicted reactant profiles for a partially-premixed opposed jet flame. CH_4 -air ($\phi=0.63$) vs. H_2 -air ($\phi=0.4$). Experimental strain rate = 258 sec^{-1} .

post flame zone and the spectrum at location 14.75 mm represents a lean H_2 -air flame zone that is only partially reacted. From these four spectra and the uncertainty calculation, it is found all laser-induced background levels are much lower than the previous results [7,8] due to improvements in the detection system.

(2) Lean, “positive flame speed” CH_4 flame versus hot products

Experimental measurements and numerical predictions of temperatures and reactants concentrations are compared in Fig. 5. Raman data could not be obtained for the inside part of the top jet, thus the x axis range starts at 0.3 cm. As seen from the experimental data, a premixed “positive flame speed” flame exists on the side of CH_4 -air mixture relative to the stagnation plane. It is found that experimental profiles of O_2 , N_2 and CH_4 match very well with numerical profiles in the CH_4 -air premixed flame zone and in the H_2 -air post flame zone. The predicted peak temperature is about 180 K lower in the premixed flame zone, although peak location is predicted correctly. There is an opposite trend for O_2 concentration profile, it is slightly over-predicted in this zone. The experimental data don’t agree well with the predicted results near the exit of the H_2 -air flame because the high laminar flame speed and low flow rate caused the flame to be partially anchored. The experimental data show there is unburned H_2 and relatively high water vapor around the exit. Based on an assumption that 40% of the mixture is burned at the nozzle exit, the boundary conditions on the H_2 -air side are calculated with Stanjan and they are as follows: H_2 : 0.087, O_2 : 0.1552, N_2 : 0.698, H_2O : 0.060 (species in mole fraction); temperature: 775K. The velocity of the mixture estimated from temperature ratio ($775/300$) is 119 cm/s. Figure 6 shows the experimental measurement and numerical predictions of product concentrations. The predicted water vapor and CO_2 have

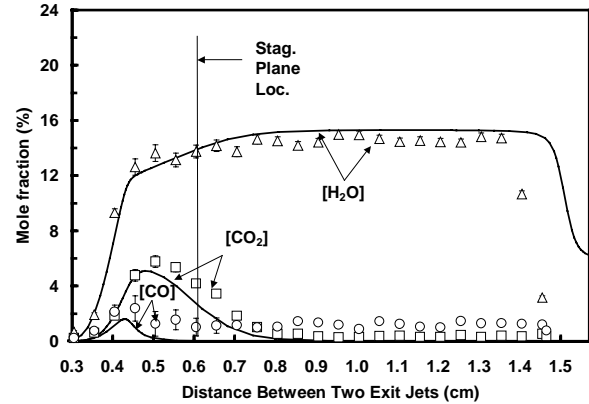


Figure 6. Experimental and numerically-predicted products profiles for a partially-premixed opposed jet flame. CH_4 -air ($\phi=0.63$) vs. H_2 -air ($\phi=0.4$). Experimental strain rate = 258 sec^{-1} .

similar profiles as the experimental data, for example, experimental CO_2 has a peak value 5.7% mole fraction, and predicted CO_2 mole fraction has value of 5.1%. Considering 7% uncertainty, they agree well. For minor species CO, the general trend is similar, but the uncertainty is higher. Compared to propane data shown in [7], this CH_4 -air “positive flame speed” flame shows much better agreement between experimental data and numerical simulation for the same boundary and initial conditions.

(3) Very lean, “negative flame speed” CH_4 flame versus hot products

Figures 7 and 8 show the experimental results and numerical predictions for a lean CH_4 -air ($\phi=0.50$) mixture impinging upon an H_2 -air jet ($\phi=0.4$). There is only a slight difference for this premixed mixture compared to the previous “positive flame speed” flame: the equivalence ratio is dropped from 0.63 to 0.5. From Fig. 8, it is found a lean CH_4 -air premixed “positive flame speed” flame doesn’t exist on the CH_4 -air side of the stagnation plane. The CH_4 Raman signal disappears around the stagnation plane, indicating that either the CH_4 fuel reacts in this zone or CH_4 is convected away at the stagnation plane. In fact, it is found there is a very weak flame that is formed by CH_4 diffusing across the stagnation plane and reacting with the excess O_2 from the H_2 -air premixed flame from the other jet. This weak flame is called a “negative flame speed” flame [10,12]. This flame is so weak that it can only be seen by eye in a dark room. There are two prerequisites for this weak flame to exist: 1) high strain rate and 2) excess oxidizer and high temperature hot products from another jet to support it.

Similarly, the H_2 -air mixture is partially burned. For this flame, it is assumed that 50% of the mixture

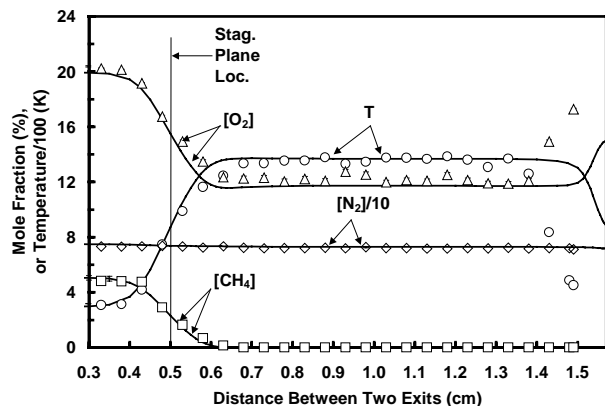


Figure 7. Experimental and numerically-predicted reactant profiles for a partially-premixed opposed jet flame. CH₄-air ($\phi=0.50$) vs. H₂-air ($\phi=0.4$). Experimental strain rate = 230 sec⁻¹.

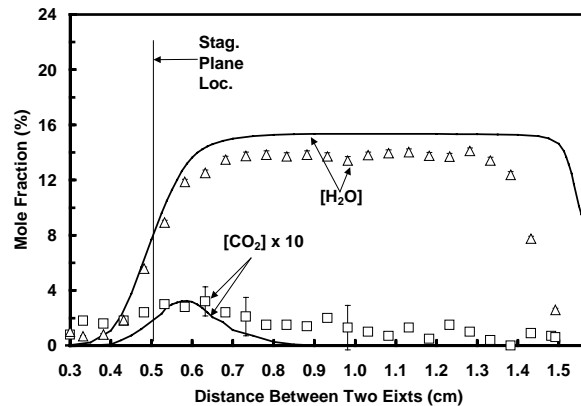


Figure 8. Experimental and numerically-predicted product profiles for a partially-premixed opposed jet flame. CH₄-air ($\phi=0.50$) vs. H₂-air ($\phi=0.4$). Experimental strain rate = 230 sec⁻¹.

is burned and the related boundary conditions on the H₂-air side are as follows: H₂: 0.074, O₂: 0.149, N₂: 0.7015, H₂O: 0.0746 (species in mole fraction); temperature: 883K. The velocity of the mixture is estimated from the temperature ratio (883/300) and gives 135 cm/s. In Fig. 7, all profiles for reactants and temperature have excellent agreement between experimental data and numerical simulation. The H₂O profile in Fig. 8 demonstrates the same trend between predicted and experimental data, but there is a 1% discrepancy in mole fraction, that is, the predicted H₂O mole fraction is higher than the experimental result. It should be noted that the CO₂ concentration is very low for this diffusion-controlled flame (below the 3000 ppm level). As mentioned earlier, the experimental data is noisy at these levels, but the experimental data and predicted results give pretty close values near the peak. The CO₂ profile indicates where the methane is consumed. Further, the relative order of magnitude of the CO₂ prediction and measurement are similar.

The comparison of CO₂ profiles between experimental and predicted data for very lean CH₄-air and C₃H₈-air flames are shown in Fig. 9. For the previously studied C₃H₈-fueled negative flame speed flame [7,8], the CO₂ predictions and measurements differed by an order of magnitude. For the very lean CH₄-air flame studied in this work, the predicted result and experimental data are of the same order. Therefore, one can conclude that the selected CH₄ mechanism does a better job of modeling than does the C₃H₈ mechanism previously used for this kind of very lean “negative flame speed” flame.

CONCLUSIONS

The flame structure of a lean partially premixed CH₄-air flame versus hot products is investigated by the Raman

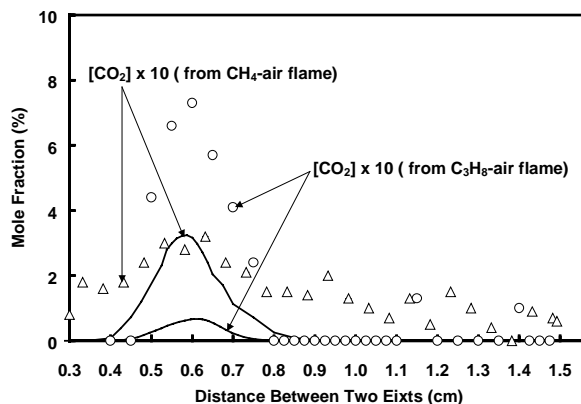


Figure 9. Comparison of CO₂ profile for two very lean hydrocarbon-air flames: CH₄-air ($\phi=0.5$) versus H₂-air ($\phi=0.4$), strain rate=230 sec⁻¹; C₃H₈-air ($\phi=0.6$) versus H₂-air ($\phi=0.4$), strain rate=390 sec⁻¹

scattering technique and numerical simulation. The understanding of this very lean mixture combustion can help to reduce the pollutants occurring in a DISI engine. An improved optical collection system gives good discrimination against flame background and laser induced background, leading to lower measurement uncertainties than previous investigation. Two typical flame structures are studied and experimental data and predicted results show very good agreement for both.

Agreement for the two flames verifies that the chosen kinetic mechanism GRI-Mech 3.0 is appropriate for these lean flames. There is no major discrepancy in the CO₂ profiles as found in a previous C₃H₈-air flame study.

The experiment and simulation both demonstrate the existence of either a lean positive flame speed flame or a very lean negative flame speed flame with

hot products impinging on lean reactants. For these flames, the effect of hot products is to maintain them.

ACKNOWLEDGEMENTS

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