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**EXPERIMENTAL AND DETAILED NUMERICAL STUDIES
OF FUNDAMENTAL FLAME PROPERTIES
OF GASEOUS AND LIQUID FUELS**

(AFOSR Grant No. FA9550-04-1-0006)

Principal Investigator: Fokion N. Egolfopoulos

Department of Aerospace & Mechanical Engineering
University of Southern California
Los Angeles, California 90089-1453

SUMMARY/OVERVIEW

The main goal of this research is to provide archival experimental data and provide insight into the physical and chemical mechanisms that control various flame phenomena for a wide range of conditions. Fuel type, equivalence ratio, flame temperature, and combustion mode are the parameters considered. The experimental data are important for a number of reasons. First, they constitute a basis for *partially* validating the combustion chemistry of a large number of fuels ranging from hydrogen to gaseous and liquid hydrocarbons and alcohols. Second, they can be used in order to assess the effect of uncertainties of diffusion coefficients on the prediction of global flame properties. Finally, such data are essential for assessing the reliability of proposed surrogates of realistic fuels, which are of relevance to air-breathing propulsion. The results and findings of this program are of immediate interest to the design and performance of advanced air-breathing propulsion devices. During the reporting period, progress was made in the following: (1) Studies of flame and ignition kinetics of dry synthesis gas mixtures; (2) Assessment of diffusion and kinetics effects on flame ignition; (3) Determination of lean flammability limits of methane/air and propane/air mixtures under engine-like conditions; (4) Determination of ignition and extinction limits of premixed and non-premixed flames for a wide range of jet and gasoline fuels and their surrogates.

TECHNICAL DISCUSSION

The studies include both experiments and detailed numerical simulations. The experiments are conducted in the opposed jet configuration that allows for the systematic determination of the fluid mechanics effects on flames and can be also modeled directly along its stagnation streamline. The experiments are performed in a variable pressure chamber. The reported measurements, were performed at $p = 1 \text{ atm}$ through the use of a Digital Particle Image Velocimetry (DPIV) technique [1] and thermocouples with appropriate corrections to account for radiative losses. The numerical simulations include the use of CHEMKIN-based codes. Several chemical kinetics schemes have been tested.

1. Studies of flame and ignition kinetics of dry synthesis gas mixtures with air

This is a collaborative effort with Professors Hai Wang of USC and Eric L. Petersen of University of Central Florida, and more details can be found in Ref. 2. The reaction kinetics of

H₂ and CO mixtures were examined experimentally and computationally under mixture and reaction conditions of immediate interest to synthesis gas combustion. Shock-tube ignition delay times were obtained for five CO-H₂-air mixtures (equivalence ratio $\phi = 0.5$) over the pressure range of 1 to 20 atm and temperatures from 950 to 1330 K. The influence of synthesis gas composition variations on flame ignition and propagation was also examined. Two types of experiments were carried out for H₂/CO/CO₂ mixtures with air. Laminar flame speeds were determined in the twin-flame counterflow configuration using Digital Particle Image Velocimetry [1]. Ignition temperatures were determined by counterflowing a vitiated air jet against a premixed fuel/air jet [3]. Computationally, detailed modeling of the experiments were performed, using a recently developed H₂/CO reaction model [4]. Numerical simulations showed generally good agreement with the experimental data.

2. Assessment of diffusion and kinetics effects on flame ignition

The relative importance of molecular transport and chemical kinetics on flame ignition was investigated through detailed numerical simulations, and more details can be found in Ref. 5. The study was conducted in stagnation-type flows for atmospheric, laminar premixed and non-premixed *iso*-C₈H₁₈, *n*-C₇H₁₆, and H₂ flames.

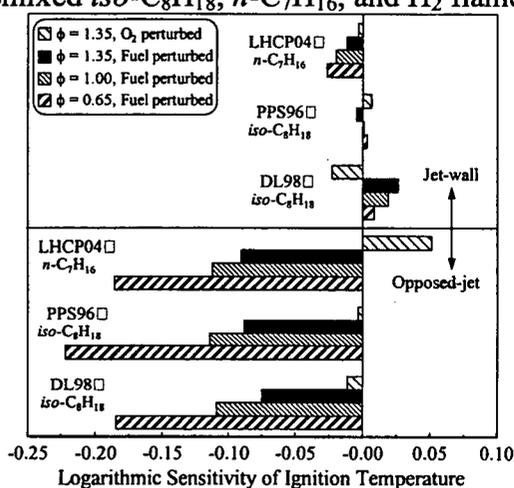


Fig. 1. Logarithmic sensitivity coefficients of ignition temperature of *iso*-C₈H₁₈/air and *n*-C₇H₁₆/air flames on diffusion.

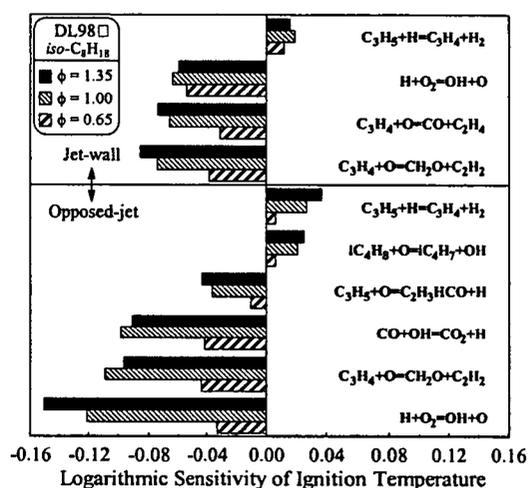


Fig. 2. Logarithmic sensitivity coefficients of ignition temperature of *iso*-C₈H₁₈/air on kinetics

Ignition of premixed flames was studied by: (1) increasing the temperature of a N₂ jet counterflowing against a fuel/air jet, (2) increasing the temperature of a solid wall against which a fuel/air jet was injected. Ignition of non-premixed flames was studied by increasing the temperature of an air jet counterflowing against a fuel-containing jet. The simulations were performed along the stagnation streamline, and included detailed descriptions of chemical kinetics, molecular transport, and radiative heat transfer. Sensitivity analyses of the ignition temperatures to the diffusion coefficients of the reactants as well as to the kinetics were performed. Results revealed that premixed flame ignition is rather sensitive to the fuel diffusivity in the opposed-jet configuration, and notably less in the jet-wall. This is due to the diffusive transport that is required to convey the reactants towards the ignition kernel in the opposed-jet. It was found that the two approaches result in similar ignition temperatures only for fuel-rich cases and that the ignition temperatures tend to be lower as the equivalence ratio increases in the opposed-jet configuration. However, the ignition temperatures were found to

depend mildly on the equivalence ratio in the jet-wall configuration. The sensitivity of ignition to diffusion in non-premixed systems was found to also be notable, especially for cases in which the fuel is highly diluted by an inert. For both premixed and non-premixed flames, the sensitivity of ignition to diffusion coefficients was found to be of the same order or larger than that to kinetics, and representative results are shown in Figs. 1 and 2. This is important when flame ignition data are used to validate kinetics, as rate constants could be potentially falsified. This has been also shown to be the case for the extinction of H₂ [6] and liquid fuel flames [7] by demonstrating that the sensitivity of the extinction limits on diffusion can be of the same or even greater order compared to that of kinetics.

3. Determination of lean flammability limits of methane/air and propane/air mixtures under engine-like conditions

This is a collaborative effort with Professor Chung K. Law of Princeton University, and more details can be found in Ref. 8. In this study, the lean flammability limits of CH₄/air and C₃H₈/air mixtures were numerically determined for a wide range of pressures and unburned mixture temperatures in order to assess the near-limit flame behavior under conditions of relevance to internal combustion engines. The study included the simulation of freely propagating flames with the inclusion of detailed descriptions of chemical kinetics and molecular transport, radiative loss, and a one-point continuation method to solve around singular points as the flammability limit is approached. Results revealed that both pressure and unburned mixture temperature have significant effects on the lean flammability limit as well as the attendant limit flame temperature. Specifically, the lean limit was found to first increase and then decrease with pressure, while the limit temperature decreases with pressure in general, and can be reduced to values as low as 900 K under engine-like conditions. Through sensitivity and species consumption path analyses it was further shown that the chain mechanisms that control the near-limit flame response critically depend on the thermodynamic state of the mixture. Thus, mechanisms that are identified as important at near-atmospheric conditions may not be relevant at higher pressures and unburned mixture temperatures. In particular, the response of near-limit flames was found to resemble the homogeneous explosion limits of hydrogen/oxygen mixtures in that while at low pressures the main branching and termination reactions are respectively $H + O_2 \rightarrow OH + O$ and $H + O_2 + M \rightarrow HO_2 + M$, at the elevated pressures relevant to internal combustion engines the system branching is controlled by the HO₂-H₂O₂ kinetics. Potential avenues for extending the lean operation limits of internal combustion engines were suggested based on the understanding gained from this analysis.

4. Determination of ignition and extinction limits of premixed and non-premixed flames for jet and gasoline fuels and their surrogates.

The jet fuels study is a collaborative effort with Dr. Tim Edwards of AFRL, and more details can be found in Ref. 9. Extinction strain rates and ignition temperatures of a wide range of jet fuels were experimentally determined in the counterflow configuration under non-premixed conditions. Similar measurements were also made for single-component hydrocarbon fuels and surrogate fuels, and were compared with those obtained for the jet fuels. The experiments were conducted at atmospheric pressure and elevated temperatures. Comparing single-component hydrocarbon fuels, it was found that those with lower carbon number exhibit greater resistance to extinction and greater ignition propensity. The results for the jet fuels revealed that there is a large variation in both extinction and ignition limits. Jet fuels with similar extinction behavior were found to display a rather different ignition response. Two recently proposed JP-8 surrogates

were also tested, and both the ignition and extinction states of a reference JP-8 fuel were not predicted satisfactorily. Both surrogates were found to exhibit a more robust combustion behavior compared to JP-8, as manifested by their increased ignition propensity and their increased resistance to extinction.

Ignition and extinction limits of samples of gasoline, mixtures of gasoline, proposed gasoline surrogates, and selected single-component liquid hydrocarbons with air, were experimentally determined in the counterflow configuration, and more details can be found in Ref. 10. The experiments were conducted at atmospheric pressure and elevated temperatures. Results revealed that different samples of gasoline exhibit notably different ignition and extinction characteristics while averaged mixtures of gasoline behave rather similarly. Comparing the single-component hydrocarbons, the lower molecular weight paraffins were found to have greater ignition propensity and reduced extinction resistance compared to the larger molecular weight ones. Comparing *n*-C₈H₁₈ and *iso*-C₈H₁₈, it was found that while *n*-C₈H₁₈ flames ignite more readily, as expected, they also exhibit greater resistance to extinction compared to *iso*-C₈H₁₈ flames.

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