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Experimental and Computational Studies of Fundamental Properties of Jet Fuel Flames at Engine-Relevant Conditions

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14. ABSTRACT
A comprehensive three-year research program was carried out on the characterization of fundamental properties of jet and rocket fuel flames under engine-relevant conditions with increased accuracy and well-defined uncertainties for the first time. The results of the proposed work contributed notably towards the development of real fuel kinetics. Specifically, the following were accomplished: (1) A newly developed approach was implemented to measure laminar flames speeds. The approach involved experiments of spherically expanding flames in constant volume vessels in tandem with direct numerical simulations that allow for the accurate characterization of stretch effects and radiation. Measurements were carried out for pressures up to 15 atm and unburned reactant temperatures up to 750 K without decomposing the fuel during the compression stage of the experiment; (2) Measurements of extinction strain rates were carried out in the counterflow configuration at 1 atm for unburned reactant temperatures up to 500 K; and (3) The data were modeled using state of the art codes and in close collaboration with the kinetics teams that are responsible for developing real fuels kinetics.

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Potential Energy Surfaces, Reaction Kinetics, and Transport Processes in High-Speed Combustion

(AFOSR Grant FA9550-15-1-0409)

(Period: September 30, 2015 – July 29, 2019)

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Summary and overview

The main goal of the completed research program was to provide fundamental flame data for conditions of relevance to air-breathing and rocket propulsion. Specific focuses were placed on three areas of research: (1) Advancing the spherically expanding flame approach for investigating laminar flame propagation for heavy liquid fuels at engine relevant conditions using modern mathematical and modeling tools; (2) Measuring with reduced uncertainty fundamental flame properties of jet and rocket fuels under thermodynamic conditions that have not been considered adequately in the past; and (3) Providing support and validation for Hybrid Chemistry (HyChem) approach for modeling high-temperature combustion chemistry of practical jet and rocket fuels.

During the reporting period, the following tasks were completed:

1. Measurements of laminar flame speeds and extinction strain rates at atmospheric pressure and elevated mixture temperatures for flames of practical propulsion fuels. The measurements were carried out in the well-established counterflow configuration.
2. Advancement of the spherically expanding flame approach under constant volume conditions was via combined modeling and experimental efforts and the associated data uncertainty has been reduced notably.

3. Implementation of the spherically expanding flame technique for measuring laminar flame speeds of practical propulsion fuels up to 15 atm and 750 K.
4. Support of the development of the HyChem kinetic models by Stanford University via systematic measurements and flame modeling.

Technical discussion

1. Background

Laminar flame ignition, propagation, extinction, and structure can be investigated at near atmospheric and elevated pressures utilizing steady-state burner configurations. However, at pressures well above 10 atm steady-state flows are susceptible to flow instabilities due to the increase in the Reynolds number (*Re*) and the fact that the burner diameter cannot be reduced below 5 mm or so in order to assure a reasonable spatial resolution with intrusive or non-intrusive diagnostics.

Laminar flame studies in steady-state experiments above 10 atm are limited. For example, Seshadri and coworkers [1][2] measured extinction strain rates (K_{ext}) of non-premixed H_2, CH_4, and C_2H_6 counterflow flames (CFF) for pressures up 20 atm. Gomez and coworkers [3][4] established non-premixed CH_4 and C_2H_6 CFFs for pressures up to 25 atm, and performed measurements of major species using a capillary probe. Additionally, laminar co-flow diffusion flames have been used to quantify sooting behavior of gaseous fuel flames at $P \leq 100$ atm [5].

In addition to issues related to *Re*, the flame thickness could decrease notably at high pressures, which, especially in premixed flames, makes flame speciation measurements rather challenging due to spatial resolution limitations resulting from the finite probe diameter size. Thus, S_u^o [6] becomes the only flame observable that can be measured with increased accuracy at engine-relevant P and T_u conditions [7] using the spherically expanding flame (SEF) method in constant volume chambers.

Over the years, S_u^o has been measured using various experimental techniques including Bunsen flames (e.g., [8]-[10]), CFFs (e.g., [11][12]), burner-stabilized flames (e.g., [13][14]), and SEFs under constant pressure (CONP) (e.g., [15]-[17]) and constant volume (CONV) conditions (e.g., [18]-[22]). While a large number of reliable S_u^o data has been produced at and near-atmospheric pressures and temperatures.

Practical liquid fuels are comprised of a large number of components and as a result modeling their kinetic behavior is a challenging task. Significant progress has been made over the years using the traditional surrogate and the recently developed HyChem approaches (e.g., [23][24]). S_u^o data at engine-relevant conditions are essential for testing combustion models, and a literature survey ([24]-[84]) on S_u^o measurements for flames of pre-vaporized neat C_7-C_{16} and jet and rocket fuels was carried out. In Fig. 1 the survey results are grouped for: (1) jet and rocket fuels; (2) neat fuels with $7 \leq C\# \leq 12$; and (3) neat fuels with $C\# > 12$, where C# is the average carbon number of the fuel.

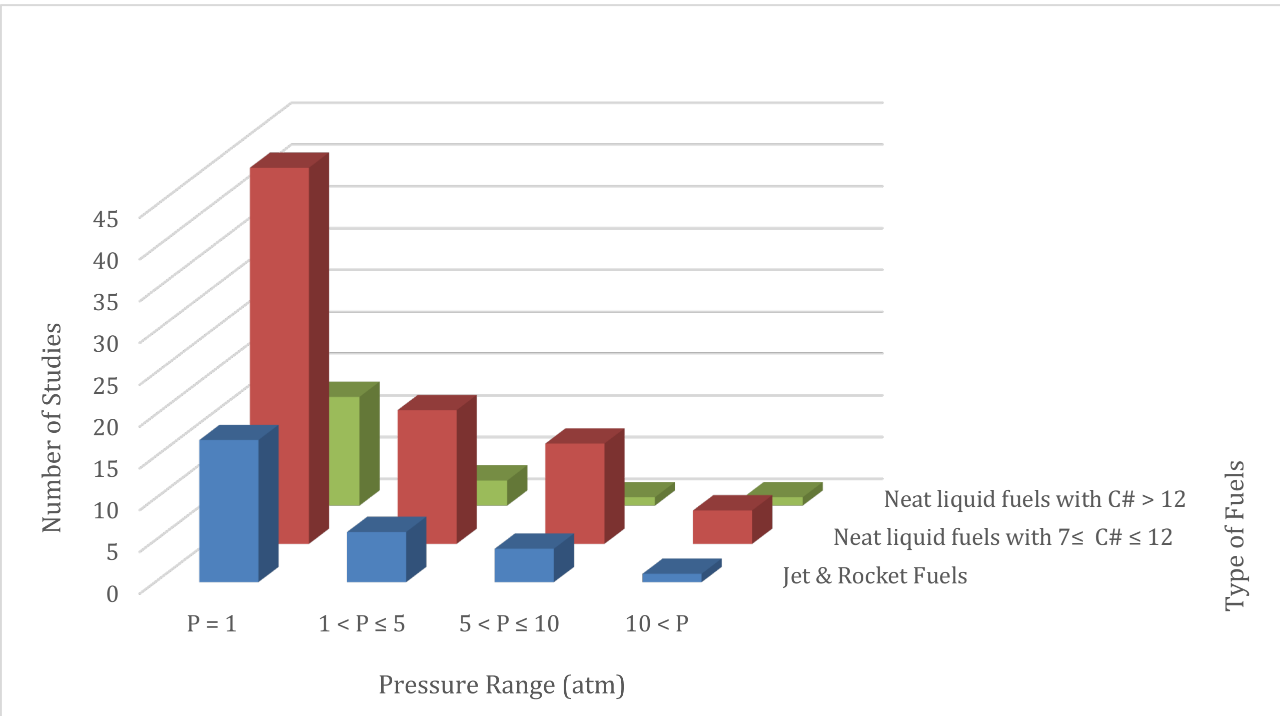

Figure 1. Number of laminar flame speed experimental studies for pre-vaporized liquid (neat and jet/rocket) fuels depicted as a function of pressure.

2. Summary of experimental and modeling efforts

2.1 Laminar flame speeds under engine-relevant conditions:

The spherically expanding flame method is the only approach for measuring laminar flame speeds at thermodynamic states that are relevant to engines. A comprehensive evaluation of data obtained under constant pressure and constant volume conditions was carried out through experiments, development of a mathematically rigorous method for uncertainty quantification and propagation, and advancement of numerical models that describe the experiments accurately. The proposed uncertainty characterization approach accounts for parameters related to all measurements, data processing, and finally data interpretation. With the aid of direct numerical simulations, an alternative approach was proposed to derive laminar flame speeds in constant pressure experiments by eliminating the need for using extrapolation equations developed on simplifying assumptions, which are known to be susceptible to major errors under certain conditions. The propagation of spherical flames under constant volume conditions was investigated through experiments carried out in an entirely spherical chamber and the use of two numerical models. The first involves the solution of the fully compressible one-dimensional conservation equations of mass, species, and energy. The second model was developed based on thermodynamics similarly to existing literature, but radiation loss was introduced at the optically thin limit and approximations were made to allow for re-absorption with minimum computational cost. It was shown that neglecting radiation in constant volume experiments could introduce errors as high as 15%. Incorporating the aforementioned techniques, laminar flame speeds were measured and reported with properly quantified uncertainties for flames of synthesis gas for pressures ranging from 3 to 30 atm, and unburned mixture temperatures ranging from 298 to 550 K. Selected measurements were carried out as well for methane and propane flames for pressures ranging from 3 to 7 atm, and unburned mixture temperature of 298 K. The approaches introduced in this study allow for the determination of laminar flame speeds with notably reduced uncertainties under conditions of relevance to engines, which has major implications for the validation of kinetic models of surrogate and real fuels.

The results have been published and can be found at:

- C. Xiouris, T. Ye, J. Jayachandran, F.N. Egolfopoulos, Laminar Flame Speeds under Engine-Relevant Conditions: Uncertainty Quantification and Minimization in Spherically Expanding Flame Experiments, ***Combustion and Flame*****, 163 (2016) 270-283**.

2.2 Near-boundary ignition behavior of reacting mixtures

The autoignition behavior is key towards providing insight into a fuel's behavior and performance and equally important towards developing kinetic models. However, there has been evidence in past literature that under certain conditions legacy reactor experiments may exhibit inhomogeneities that could potentially reduce the scientific value of the reported data. In this study, detailed one-dimensional simulations were carried out in order to provide additional insight into the aforementioned observations. The main focus of the present investigation is on the effects of a colder wall relatively to the core of the reacting mixture, and the attendant development of thermal boundary layers. It is determined that the thermal stratification could alter the ignition behavior for fuels that exhibit distinct negative temperature coefficient behavior and could cause also light and heavy species concentration stratification due to Ludwig-Soret diffusion. More specifically, simulations performed for *n*-heptane/air mixtures revealed that localized exothermic centers could develop for a range of initial mixture temperatures. Furthermore, simulations for hydrogen/oxygen/argon mixtures showed that species stratification caused by Ludwig-Soret diffusion could lead to increased local heat release rates.

The results have been published and can be found at:

- J. Jayachandran, F.N. Egolfopoulos, Thermal and Ludwig-Soret diffusion effects on near-boundary ignition behavior of reacting mixtures, ***Proceedings of the Combustion Institute*** **36 (2017) 1505-1511**.

2.3 Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes

This study resolved the experimental and modeling discrepancies previously observed for the extinction strain rates of counterflow, non-premixed n-decane and n-dodecane/nitrogen mixture versus oxygen. To achieve this goal, a recently developed transport theory of cylindrical molecular structure in dilute gases is used to model the binary diffusion coefficients of long-chain n-alkanes up to *n*-dodecane in N_2 and He. The updated diffusion coefficients are found to be significantly different from early estimates made from the law of corresponding states. The diffusion coefficient update removes the early difficulties in modeling the extinction strain rates for non-premixed extinction of *n*-decane and *n*-dodecane. It was found that the mixture averaged transport formulation can provide good predictions provided that the Soret effect on the transport of large fuel molecules is properly accounted for.

The results have been published and can be found at:

- C. Liu, R. Zhao, R. Xu, F.N. Egolfopoulos, H. Wang, Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes, ***Proceedings of the Combustion Institute*** **36 (2017) 1523-1530**.

2.4 A physics-based approach to modeling real-fuel combustion chemistry (HyChem)

Real distillate fuels usually contain thousands of hydrocarbon components. Over a wide range of combustion conditions, large hydrocarbon molecules undergo thermal decomposition to form a small set of low molecular weight fragments. In the case of conventional petroleum-derived fuels, the composition variation of the decomposition products is washed out due to the principle of large component number in real, multicomponent fuels. From a joint consideration of elemental conservation, thermodynamics and chemical kinetics, it is shown that the composition of the thermal decomposition products is a weak function of the thermodynamic condition, the fuel-oxidizer ratio and the fuel composition within the range of temperatures of relevance to flames and high temperature ignition. Based on these findings, a hybrid chemistry (HyChem) approach was explored towards the modeling the high-temperature oxidation of real, distillate fuels. In this approach, the kinetics of thermal and oxidative pyrolysis of the fuel is modeled using lumped kinetic parameters derived from experiments, while the oxidation of the pyrolysis fragments is described by a detailed reaction model. In support of this major effort in reaction kinetics, measurements of laminar flame speeds up to 15 atm and 750 K were carried out using the constant volume spherically expending flame method for: (1) Jet and rocket fuels; (2) JP10; and (3) Bio-derived jet fuel and its blends with a conventional Jet A.

The results have been published and can be found at:

- H. Wang, R. Xu, K. Wang, C.T. Bowman, R.K. Hanson, D.F. Davidson, K. Brezinsky, F.N. Egolfopoulos, A physics-based approach to modeling real-fuel combustion chemistry - I. Evidence from experiments, and thermodynamic, chemical kinetic and statistical considerations, ***Combustion and Flame*, 193 (2018) 502-519**.
- R. Xu, K. Wang, S. Banerjee, J. Shao, T. Parise, Y. Zhu, S. Wang, A. Movaghar, D.J. Lee, R. Zhao, X. Han, Y. Gao, T. Lu, K. Brezinsky, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang, A physics-based approach to modeling real-fuel combustion chemistry - II. Reaction kinetic models of jet and rocket fuels, ***Combustion and Flame* 193 (2018) 520-537**.
- Y. Tao, R. Xu, K. Wang, J. Shao, S.E. Johnson, A. Movaghar, X. Han, J-W. Park, T. Lu, K. Brezinsky, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang,

A physics-based approach to modeling real-fuel combustion chemistry - III. Reaction kinetic models of JP10, ***Combustion and Flame*** **198 (2018) 466-476**.

- K. Wang, R. Xu, T. Parise, J. Shao, A. Movaghar, D.J Lee; J.-W, Park, Y. Gao, T. Lu, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang, A physics-based approach to modeling real-fuel combustion chemistry - IV. HyChem modeling of combustion kinetics of a bio-derived jet fuel and its blends with a conventional Jet A, ***Combustion and Flame*** **198 (2018) 477-489**.

2.5 Laminar flame propagation into a reacting mixture

The laminar flame speed is an important property of a reacting mixture and it is used extensively for the characterization of the combustion process in practical devices. However, under engine-relevant conditions considerable reactivity may be present in the unburned mixture, introducing thus challenges due to couplings of auto-ignition and flame propagation phenomena. In this study, the propagation of transient, one-dimensional laminar flames into a reacting unburned mixture was investigated numerically in order to identify the parameters influencing the mass burning rate in the conduction-reaction controlled regime at constant pressure. It was found that the fuel chemical classification significantly influences the burning rate. More specifically, for hydrogen flames, the "evolution" of the burning rate does not depend on the initial unburned mixture temperature. On the other hand, for *n*-heptane flames that exhibit low temperature chemistry, the burning rate depends on the instantaneous temperature and composition of the unburned mixture in a coupled way. A new approach was developed allowing for the decoupling of the flame chemistry from the ignition dynamics as well as for the decoupling of parameters influencing the burning rate, so that meaningful sensitivity analysis could be performed. It was determined that the burning rate is not directly affected by fuel specific reactions even in the presence of low temperature chemistry whose effect is indirect through the modification of the reactants composition entering the flame. The controlling parameters include but not limited to mixture conductivity, enthalpy, and the species composition evolution in the unburned mixture.

The results have been published and can be found at:

- A. Ansari, J. Jayachandran, F.N. Egolfopoulos, Parameters influencing the burning rate of laminar flames propagating into a reacting mixture, ***Proceedings of the Combustion Institute*** **37 (2019) 1513-1520**.

2.6 Effect of unsteady pressure rise on flame propagation and near-cold-wall ignition

Thermodynamic pressure variations during combustion can be encountered in various types of engines. Yet, hardly any studies have been conducted to investigate the effects of transient pressure rise on flame propagation as well as on the ignition of the unburned gas. In this study, the effects of unsteady pressure rise were parametrically studied using a one-dimensional reacting flow model in which the thermodynamic pressure variation is an independent variable and thus its rate of rise can be controlled. It was determined that large rates of pressure rise can significantly increase the mass burning flux of a laminar flame and that this modification becomes more pronounced at higher pressure and temperature conditions. Furthermore, it was shown that the development of ignition near a cold wall, for mixtures that exhibit negative temperature coefficient behavior, is very sensitive to rate of change of pressure. The near-wall ignition behavior was found also to be rather sensitive to the prevailing pressures and temperatures whose values control whether ignition will occur in the main-gas or within the thermal boundary layer.

The results have been published and can be found at:

- J. Jayachandran, F.N. Egolfopoulos, Effect of unsteady pressure rise on flame propagation and near-cold-wall ignition, ***Proceedings of the Combustion Institute*** **37 (2019) 1639-1646**.

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4. Personnel

This research was performed by the PI, one Research Associate (Jagan Jayachandran), and four graduate students (Chris Xiouris, Tailai Ye, Runhua Zhao, Ashkan Movaghar).

5. Archival Publications

1. C. Xiouris, T. Ye, J. Jayachandran, F.N. Egolfopoulos, Laminar Flame Speeds under Engine-Relevant Conditions: Uncertainty Quantification and Minimization in Spherically Expanding Flame Experiments, ***Combustion and Flame*, 163 (2016) 270-283**.
2. J. Jayachandran, F.N. Egolfopoulos, Thermal and Ludwig-Soret diffusion effects on near-boundary ignition behavior of reacting mixtures, ***Proceedings of the Combustion Institute* 36 (2017) 1505-1511**.
3. C. Liu, R. Zhao, R. Xu, F.N. Egolfopoulos, H. Wang, Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes, ***Proceedings of the Combustion Institute* 36 (2017) 1523-1530**.
4. H. Wang, R. Xu, K. Wang, C.T. Bowman, R.K. Hanson, D.F. Davidson, K. Brezinsky, F.N. Egolfopoulos, A physics-based approach to modeling real-fuel combustion chemistry - I. Evidence from experiments, and thermodynamic, chemical kinetic and statistical considerations, ***Combustion and Flame*, 193 (2018) 502-519**.
5. R. Xu, K. Wang, S. Banerjee, J. Shao, T. Parise, Y. Zhu, S. Wang, A. Movaghar, D.J. Lee, R. Zhao, X. Han, Y. Gao, T. Lu, K. Brezinsky, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang, A physics-based approach to modeling real-fuel combustion chemistry - II. Reaction kinetic models of jet and rocket fuels, ***Combustion and Flame* 193 (2018) 520-537**.
6. Y. Tao, R. Xu, K. Wang, J. Shao, S.E. Johnson, A. Movaghar, X. Han, J-W. Park, T. Lu, K. Brezinsky, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang, A physics-based approach to modeling real-fuel combustion chemistry - III. Reaction kinetic models of JP10, ***Combustion and Flame* 198 (2018) 466-476**.
7. K. Wang, R. Xu, T. Parise, J. Shao, A. Movaghar, D.J Lee; J.-W, Park, Y. Gao, T. Lu, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, H. Wang, A physics-based approach to modeling real-fuel combustion chemistry - IV. HyChem modeling of combustion kinetics of a bio-derived jet fuel and its blends with a conventional Jet A, ***Combustion and Flame* 198 (2018) 477-489**.
8. A. Ansari, J. Jayachandran, F.N. Egolfopoulos, Parameters influencing the burning rate of laminar flames propagating into a reacting mixture, ***Proceedings of the Combustion Institute* 37 (2019) 1513-1520**.
9. J. Jayachandran, F.N. Egolfopoulos, Effect of unsteady pressure rise on flame propagation and near-cold-wall ignition, ***Proceedings of the Combustion Institute* 37 (2019) 1639-1646**.

6.0 Interactions/Transitions

Presentations at Meetings and Conferences

1. J. Jayachandran, F.N. Egolfopoulos, Thermal and Ludwig-Soret diffusion effects on near-boundary ignition behavior of reacting mixtures, 36th International Symposium on Combustion, Seoul, Korea, July 31 – August 5, 2016.
2. C. Liu, R. Zhao, R. Xu, F.N. Egolfopoulos, H. Wang, Binary diffusion coefficients and non-premixed flames extinction of long-chain alkanes, 36th International Symposium on Combustion, Seoul, Korea, July 31 – August 5, 2016.
3. A. Ansari, J. Jayachandran, F.N. Egolfopoulos, Parameters influencing the burning rate of laminar flames propagating into a reacting mixture, 37th International Symposium on Combustion, Dublin, Ireland, July 29 – August 3, 2018.
4. J. Jayachandran, F.N. Egolfopoulos, Effect of unsteady pressure rise on flame propagation and near-cold-wall ignition, 37th International Symposium on Combustion, Dublin, Ireland, July 29 – August 3, 2018.
5. A. Movaghar, R. Lawson, F.N. Egolfopoulos, Experimental Investigations of Laminar Flame Propagation of C_1-C_4/O_2/Inert Mixtures at Engine-Relevant Conditions, paper 2F03, *11th US Combustion Meeting*, Pasadena, California, March 25-27, 2019.
6. V. Gururajan, R. Lawson, A. Movaghar, and F.N. Egolfopoulos, Using Confined Spherically Expanding Fames to Study Autoignition of Reacting Mixtures, paper 2F08, *11th US Combustion Meeting*, Pasadena, California, March 25-27, 2019.

Technical Interactions with AFRL Researchers

Several meetings with AFRL personnel took place during the reporting period during the various contractors' meetings. The purpose of these meetings was to discuss the relevance of our measurements to the Air Force related applications and identify additional needs for a variety of