PP03: HEAT RELEASE MARKERS FOR THE COMBUSTION OF ALTERNATIVE AVIATION FUELS IN GAS TURBINES

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Abstract. The aviation sector has been looking into alternative fuels in order to cope with the growing air transport demand and to moderate environmental concerns. Significant research is conducted on the characterization of various synthetic fuels. These fuels are complex mixtures of components of different chemical classes and the understanding of their combustion characteristics requires the implementation of chemical kinetic based methodologies to delineate any synergistic effects. Heat release rate is a important fundamental flame property that largely characterizes the overall combustion process. Heat release distribution in practical combustors, such as gas turbines, is crucial, not only for the identification of energy intensive flame regions, but also for the understanding and prediction of thermo-acoustic instabilities. There is considerable interest in formulating practical correlations for quantifying heat release rate in flames via appropriate chemical markers, mainly due to difficulties in obtaining a direct estimation of the former. Earlier studies performed in methane/air flames, have identified correlations between suitable kinetic information and heat release rate. However, such correlations are inadequate for unsaturated fuels under rich conditions and for oxygenated fuels under most conditions. The objective of the present work is to investigate the validity and applicability of correlations developed for methane to the combustion of other generic classes of hydrocarbons including alternative and oxygenated fuels and to underline a methodological approach for the development of more general correlations. Proposed correlations are assessed on the basis of species, elementary reaction and heat release rate data from burner-stabilized premixed flames using validated detailed kinetic mechanisms.

Keywords: Chemical kinetic markers; Heat-release rate; Laminar premixed flames; Phenomenological correlation; Practical combustors

INTRODUCTION

Heat release rate is a highly important fundamental flame property that largely characterizes the energetic outcome of the overall combustion process. Heat release distribution in practical combustors is crucial, not only for the identification of energy intensive flame regions, but also for the understanding and prediction of thermo-acoustic instabilities, pulsed combustion and combustion noise (e.g. Hardalupas et al., 2010). Direct measurement of temporally and spatially resolved heat release rate (HRR) in combustion devices is currently timely, costly and impractical. A way to overcome this problem is to formulate versatile correlations between HRR and appropriate chemical markers that can be experimentally determined with acceptable accuracy. Several such correlations have been proposed in the literature and they invariably correlate suitable detailed kinetic information (e.g. species mole fraction and/or elementary reaction rates) to the HRR in fundamental flame environments. Currently, the most reliable approach for HRR quantification involves reaction-rate imaging combining simultaneous CH_2O and OH LIF measurements. The approach has been shown to yield excellent correlations mainly in laminar and turbulent premixed methane flames but its validity for other fuels is currently unclear and has been recently questioned on the basis of experimental and numerical investigations (e.g. Kathrotia et al., 2012).

Alternative aviation fuels are composed of different hydrocarbons, the amount and type of which can differ considerably. Arguably, the composition of the fuel will affect its suitability and performance. Currently, synthetic fuels can be obtained from fossil (coal, gas) and renewable sources (waste, biomass) by many pathways including, among others, gasification applying the Fischer–Tropsch (FT) process, liquefaction, pyrolysis, hydrogenolysis and esterification, etc. Fuel composition consists of a large variety of different species belonging mainly to four chemical families: (i) long-chained unbranched alkanes (n-alkanes), (ii)

long-chained, branched alkanes (iso-alkanes) (iii) cyclo-alkanes (naphthenes) and (iv) aromatics (Braun-Unkhoff et al., 2016).

The present work summarizes and extends previous work by the authors (Gazi et al., 2013) and aims to discuss the applicability of the therein proposed methodology to novel aviation fuels. The objective of the present work is to investigate the validity and applicability of correlations developed for methane to the combustion of other generic classes of hydrocarbons including alternative and oxygenated fuels and to underline a methodological approach for the development of more general correlations. Correlations are assessed on the basis of species, elementary reaction and heat release rate data from burner-stabilized laminar premixed flames utilizing a comprehensive detailed chemical kinetic mechanism.

DEVELOPMENT OF A FLAME DATABASE AND NUMERICAL METHODOLOGY

Although real working conditions of practical combustion devices are characterized by complex flow and chemistry interactions, the validity of any correlation between HRR and appropriate chemical marker needs to be established in a well-controlled environment. A simple but yet realistic fundamental configuration suitable for the application of detailed chemistry is the laminar premixed flame. In the present work flames of different fuel classes, as well as fuel mixtures, have been considered in order to take into account the effect of isomeric structure and the interaction between single, double and triple bonds on HRR patterns. Computations have been performed with CHEMKIN (Reaction Design, 2006).

Table 1 Database of laminar premixed flames considered in the present work (please refer to Gazi et al. 2013 for complete information about flame properties)

#	Reactants (%)		#	Reactants (%)	
A	Methane	1.00	K	Acetylene	2.00
B	Methane (80%) Benzene (20%)	1.00	L	Ethylene	1.90
C	Methane (83%) Allene (17%)	1.25	M	Ethylene	2.00
D	Methane (83%) Propyne (17%)	1.25	R	Benzene	0.70
E	Methanol	0.89	S	Benzene	1.00
F	Ethanol	1.00	T	Benzene	1.78
G	Ethanol	1.00	U	Benzene	1.80
H	Ethanol	1.96	V	Benzene	2.00
I	Ethanol	2.57	W	Benzene	2.00
J	Acetylene	2.40	X	Acetylene (80%) Benzene (20%)	2.00

METHANE FLAMES

The first part of the paper provides evidence on the validity of literature correlations for laminar premixed methane flames. Figure 1a presents computed correlations between the overall heat release rate and the product of formaldehyde and hydroxyl radical concentrations in Flame A, while Fig. 1b shows the corresponding correlation for the net rate of the CH_3+O reaction. It is clear that the latter correlation is superior. Interestingly enough correlations involving the CH_2O and OH species appear to perform slightly better in the doped methane Flames B-D. However, it can generally be argued that both literature-proposed correlations are more than acceptable.

METHANOL AND ETHANOL FLAMES

The next step in the investigation relates to methanol and ethanol flames. The choice of methanol has been based on a number of reasons; it is the simplest alcohol, it has a very similar structure to methane and is adequately experimentally characterized. Furthermore, is considered as an alternative fuel by itself. It should be expected that the HRR correlations shown to be valid for methane flames, would also

be adequate for methanol flames. However, this is not the case as demonstrated in Fig. 3a. Moving further to a higher alcohol, we observe that no such simple correlations can be found for ethanol flames particularly under fuel rich conditions (Fig. 3b).
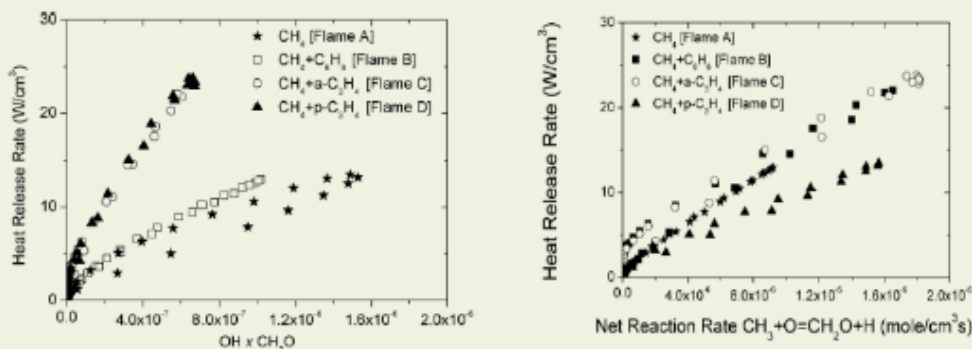

Figure 1. Correlation between HRR and (a) the product of CH₂O and OH mole fractions and the net rate of the CH₃+O reaction in flames A–D
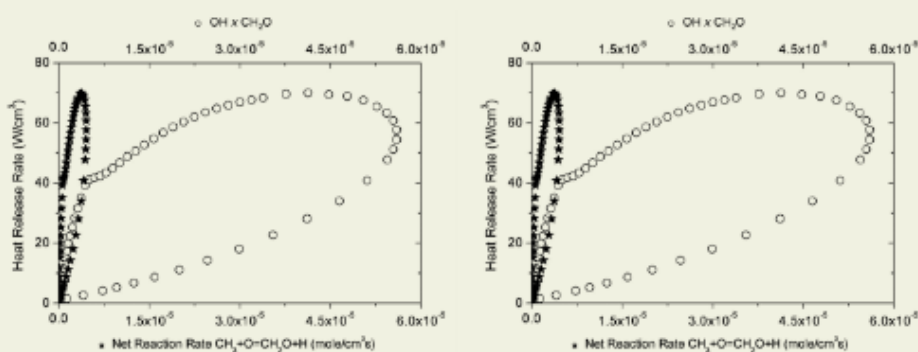

Figure 3. Correlation between HRR and (a) (i) the product of CH₂O and OH mole fractions and (ii) the net rate of the CH₃+O reaction, flame E (b) the product of CH₂O and OH mole fractions, flames G-I.

HIGHER HYDROCARBONS

Acetylene is a major intermediate in hydrocarbon flames and its chemistry is crucial for both heat release and molecular growth paths. Initial fuel consumption paths involve mainly O and OH addition reactions. The former lead to HCCO and triplet methylene radical while the later predominately lead to ketene, which subsequently is also consumed to the ketyl radical. This analysis outlines the crucial role of the ketyl radical in acetylene chemistry. Thus, Fig. 4a, [HCCO]*[O₂] is an excellent HRR marker, while the formaldehyde conjecture is not. Whether such arguments collectively characterize C₂ fuels has been also investigated. In the case of ethylene the formaldehyde correlation cannot be totally disregarded, although is not the most appropriate. On the contrary, the [HCCO]*[O₂], results in a very good probe, see Fig. 4b. Since the aromatic context in a jet fuel varies, lean to near-sooting benzene flames have been studied herein. The correlation between HRR and the product of CH₂O and OH concentrations is satisfactory, Fig. 5a. The major carbon flow in benzene flames involves initial fuel destruction to the phenyl radical, molecular oxygen attack on the latter, leading to phenoxy radical, followed by expulsion of a CO molecule and formation of cyclopentadienyl radical. Ring opening occurs through cyclopentadiene decomposition to the allyl radical and acetylene. Acetylene is then predominantly consumed to the ketyl radical, even under fuel-lean environments. Thus, the ketyl radical correlation is expected to work not only under rich conditions but also in leaner mixtures, as shown in Fig. 5b.

CONCLUSIONS

The current paper provides an appraisal of appropriate chemical markers for heat release rate correlations. Proposed correlations are assessed on the basis of species, elementary reaction and heat release rate data from burner stabilized laminar premixed flames computed utilizing a comprehensive detailed kinetic

mechanism. It is shown that correlations involving the methyl radical→formaldehyde→formyl radical pathway are adequate for methane flames and only for some lean-to-stoichiometric hydrocarbon flames. This is definitely not the case for oxygenated fuels and particularly under rich conditions. Correlations based on major carbon flow paths seem to work for relatively simple fuels. Generic correlations for rich combustion involving markers related to acetylene breakdown chemistry e.g. the $HCCO+O_2$ correlation have also been preliminary assessed.
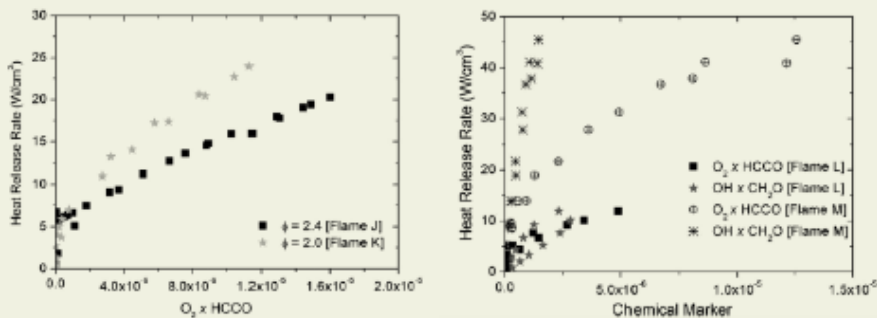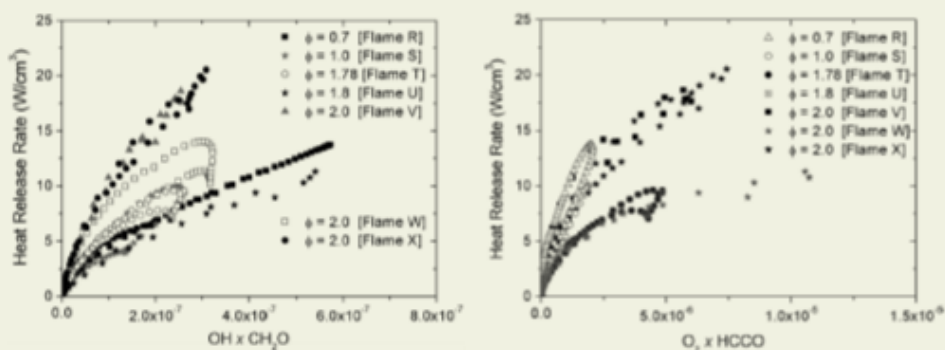

Figure 4. Correlation between HRR and (a) the product of HCCO and O_2 mole fractions for flames J and K (b) the products of $HCCOxO_2$ and CH_2OxOH mole fractions for flame L and flame M.

Correlation between HRR and (a) the product of CH_2O and OH mole fractions and (b) the product of O_2 and HCCO mole fractions for flames R–X.

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