

A Study of Flame Observables in Premixed Methane-Air Flames

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Abstract

We use a compilation of results from numerical computations of the interaction of a premixed methane-air flame with a two-dimensional counter-rotating vortex pair using detailed chemical kinetics. The investigation involves the use of two different chemical mechanisms, a two-fold variation in flow time scales, and the examination of both stoichiometric and rich methane-air flames. Correlations between a number of flame observables and heat release and burning rates are examined. We study HCO , $\nabla \cdot \mathbf{v}$, OH , CH , CO , CH_3 , CH_2O , CH_2^* , and C_2H_2 , as well as various concentration products (surrogates for production rates) including $[\text{OH}][\text{CH}_2\text{O}]$, $[\text{OH}][\text{CH}_4]$, and $[\text{OH}][\text{CO}]$. Other concentration products expected to relate to chemiluminescent observables such as CH^* , OH^* and CO_2^* are also studied. Based on the computed correlations, we comment on the utility of each observable as a measure of flame burning and heat release rates. In general, HCO mole fraction is found to have the best correlation with these rates for all cases studied.

Introduction

Proper evaluation of the performance of combustion systems requires accurate experimental determination of local flame burning and heat release rates. However, these rates are not directly measureable. Rather, specific observable flame parameters are typically measured and used to infer their values. This necessary approach assumes an implicit correlation between the particular flame observable and the rate quantity in question. Detailed computations of flame-flow interaction are useful for investigating the quality of these correlations, and for highlighting the utility of specific observables that are found to offer good correlations.

This was done first by Najm *et al.* [1], where the adequacy of certain observables as measures of flame burning and heat release rates was evaluated using both numerical and experimental data. A key result was the demonstration of the utility of HCO as a reliable flame marker and as a measure of local flame burning and heat release rates. More recently, Paul and Najm [2] found that both peak HCO concentration and the concentration product $[\text{OH}][\text{CH}_2\text{O}]$ are good measures of flame heat release rate w_T at either stoichiometric or rich conditions. The relatively easier task of PLIF imaging of OH and CH_2O concentrations, versus that of HCO , highlights the utility of the concentration product approach.

In the present work (see also [3]), we extend the above studies to investigate these and other flame observables under a wider range of flame, flow, and model parameters. We investigate correlations of HCO , $\nabla \cdot \mathbf{v}$, OH , CH , CO , CH_3 , CH_2O , CH_2^* , and C_2H_2 with flame heat release and burning rates. We also evaluate correlations of peak concentration products $[\text{OH}][\text{CH}_2\text{O}]$, $[\text{OH}][\text{CO}]$, $[\text{OH}][\text{CH}_4]$, and others associated with the production of excited species OH^* , CH^* , and CO_2^* with peak w_T . We consider a range of flow time scales, and utilize stoichiometric and rich reactants mixtures. We use both C_1 and C_1C_2 kinetic mechanisms and cross-compare predictions from the two classes of mechanisms.

The governing equations are based on the low Mach number approximation in an open domain [4, 5]. Some of the main features are the inclusion of variable transport and thermodynamic properties and detailed chemical kinetics, and the neglect of radiation and Soret and Dufour effects. The numerical construction utilizes second-order spatial and temporal discretizations, and is based on a predictor-corrector formulation of the projection method [7]. Depending on the chemical mechanism considered, and the associated stiffness of the resulting governing equations, a stiff or non-stiff version of this scheme is used. The non-stiff version is presented in detail in [4]. The stiff version, which employs a semi-implicit formulation of the scalar conservation equations is discussed in [5]. A second-order symmetric operator-split construction is also used, coupled with the semi-implicit stiff implementation, when relatively slower flows and longer interaction times are considered [6].

Results

We study the interaction of a premixed methane-air flame, 20% N₂-diluted, with a counter-rotating vortex pair in 2D, under atmospheric pressure conditions. Several flow-flame cases are considered. These include fast and slow vortex-pairs, stoichiometric and rich ($\Phi = 1.2$) reactants, and both C₁ [8] and C₁C₂ [9] (GRImech1.2) mechanisms.

A typical flow evolution is illustrated in Figure 1. The flame propagates downward, in the negative y direction, by burning into the reactants. Simultaneously, the vortex-pair propagates upward, causing contortion of the flame. The Damköhler number (Da), defined as the ratio of the vortex-pair time scale to the flame time scale, is in the range 0.02-0.3. With $Da < 1$, the flow is faster than the flame, and some flame contortion is expected. The vorticity contours in the figure illustrate the generation of a baroclinic vorticity dipole, consistent with earlier work [10]. The detailed study of the computed flame-flow interaction is outside the present scope (see [4]), rather we focus on the investigation of flame observables.

By extracting internal flame structure information along flame normal sections, we compile statistics of relevant peak mole fraction and reaction rate quantities. These are then used to examine correlations between specific flame observables and heat release and burning rates. Typical correlation plots for HCO and CH, based on various flow cases, are shown in Figure 2. These plots indicate the utility of peak HCO, versus CH, as a measure of local heat release rate, for the range of operating parameters considered. While some degradation of correlation due to variation in equivalence ratio from 1.0 to 1.2 is evident in the HCO data, this degradation is more severe for CH, along with significant scatter due to flow unsteadiness. The rich flame peak CH mole fraction is found to be higher than that in the stoichiometric flame, but at lower peak w_T . The two data sets merge at low heat release rate as the flame approaches extinction. While each of the stoichiometric and rich flame data may be used to construct a local correlation, no generally good correlation is feasible. Therefore, the use of peak CH to infer heat release and burning rate requires knowledge of the local flame stoichiometry. This information may not be readily available in a general turbulent reacting flow. In this sense, we conclude that the utility of peak CH as a measure of local heat release and burning rates is adversely affected by its dependence on equivalence ratio.

Similar data has been acquired for a range of other observables, as indicated earlier. This material is not included here due to space limitations. However, some conclusions, again pertinent to the present flow-flame conditions, are as follows:

1. Peak $\nabla \cdot \mathbf{v}$, and CO mole fraction gradient, correlation with heat release rate is adversely affected by scatter due to flow unsteadiness. In the case of CO gradient, this is primarily due to the relative stability of CO. As for $\nabla \cdot \mathbf{v}$, this scatter is due to the effect of flow unsteadiness on heat diffusion fluxes in the flame. As observed in [1], the dominant contributions to $\nabla \cdot \mathbf{v}$ are those due to heat release rate w_T and the diffusion of heat $\nabla \cdot (\lambda \nabla T)$. Flow unsteadiness effects on $\nabla \cdot (\lambda \nabla T)$ can lead to observations of peak $\nabla \cdot \mathbf{v}$ varying inversely with w_T .
2. Peak OH, CH₃, CO, and CH mole fraction correlations with w_T are adversely affected by their specific dependence on equivalence ratio.
3. Peak CH₂O correlation with w_T is very good at low heat release rate, with no adverse dependence on equivalence ratio. On the other hand, its sensitivity to changes in w_T is minimal at high heat release rates.
4. Peak CH₂* was found to exhibit reasonable correlation with peak w_T , albeit with significant scatter.
5. Peak concentration products [OH][CH₄], [OH][CO], and [CO][O] (a possible surrogate for CO₂* production rate) exhibit good correlation with w_T , with some scatter.
6. Peak [C₂H][O] (a possible surrogate for CH* production rate) exhibits significant scatter due to flow unsteadiness.
7. Peak [CH][O₂] (a possible surrogate for OH* production rate) is very well correlated with w_T .
8. Peak [OH][CH₂O] exhibits good correlation with w_T with little scatter but some adverse dependence on equivalence ratio.

9. HCO is an excellent flame marker and measure of burning and heat release rates for all the cases considered, with little adverse dependence on equivalence ratio. This is true both for point-to-point and peak-to-peak correlation studies.

Closing Remarks

In closing, it is important to note that these findings are necessarily specific to the range of flow and flame parameters investigated, the chemical mechanisms considered, and the presumed methane-air fuel mixture. Additional work is necessary to evaluate their extension to wider ranges of operating conditions, or to other fuels and mixture compositions. On the other hand, the results suggest clearly the need for demonstration of the utility of specific flame observables before they are used in experimental measurements of flames as measures of overall burning or heat release rate.

Acknowledgments

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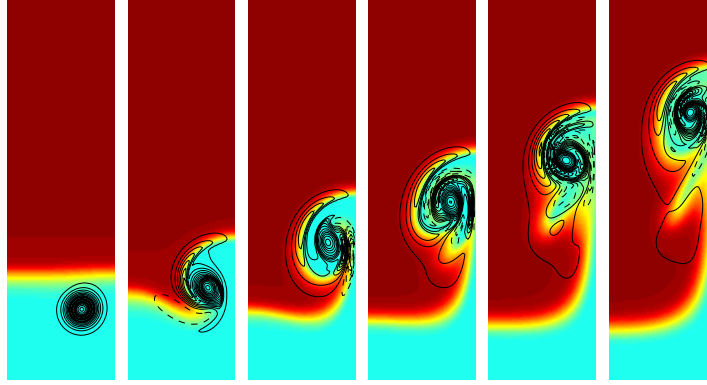


Fig. 1. Time sequence illustrating computed flame interaction with the counter-rotating vortex-pair. The vertical right-hand-side edge of each frame is the vortex-pair centerline. The time span is 1.0 ms, left to right, with an interval between adjacent frames of 0.2 ms. The shading indicates gas temperature, with the unburnt reactants at the bottom. The solid/dashed contours delineate levels of positive/negative vorticity.

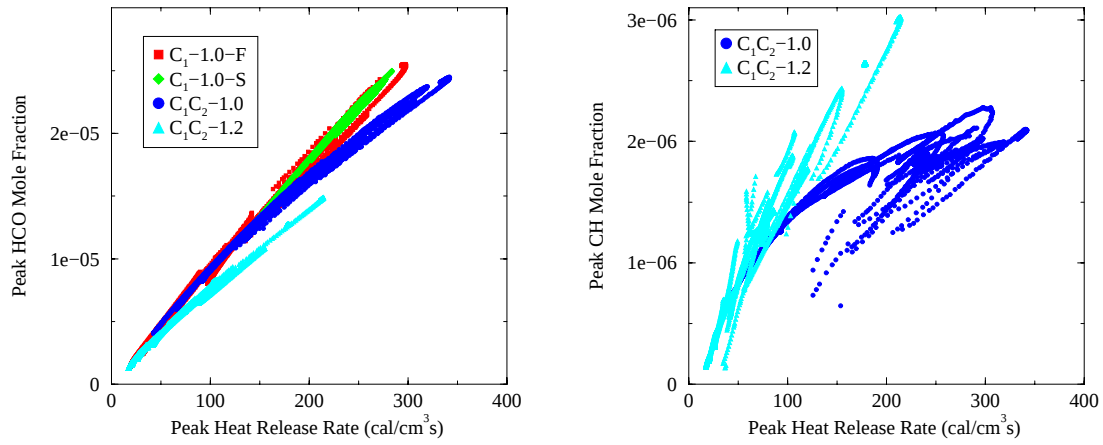


Fig. 2. Peak-to-peak correlation between HCO and CH mole fractions, and flame heat release rate.