

# Supersonic Combustion Simulation of Cavity-Stabilized Hydrocarbon Flames using Ethylene Reduced Kinetic Mechanism

P. Gokulakrishnan<sup>1</sup>, S. Pal<sup>2</sup>, M. S. Klassen<sup>3</sup>, A. J. Hamer<sup>4</sup> and R. J. Roby<sup>5</sup>  
*Combustion Science & Engineering, Inc.*  
8940 Old Annapolis Road, Suite L, Columbia, MD 21045

O. Kozaka<sup>6</sup> and S. Menon<sup>7</sup>  
*School of Aerospace Engineering*  
*Georgia Institute of Technology, Atlanta, GA 30332*

Hydrocarbons become viable alternatives to hydrogen at Mach numbers below 10, because of greater fuel densities and endothermic cooling capabilities. However, hydrocarbons show difficulties for flame holding under supersonic conditions due to their long ignition delay times. Thus, developing reduced kinetic models that are capable of predicting ignition and blow-out becomes a challenge at scramjet conditions. In the present approach, the fuel molecule breaks-down into CH<sub>2</sub>O and H<sub>2</sub> and a detailed CH<sub>2</sub>O/H<sub>2</sub>/O<sub>2</sub> reaction subset consisting of 14 species and around 40 reactions is used for accurate predictions. Using this approach reduced kinetic models for ethylene was developed. Also, the application of this reduced kinetic model for scramjet simulation was demonstrated by implementing in a RANS code to predict combustion stability in a cavity flameholder experiments. The reduced model was able predict the stable and lean blowout experimental conditions reasonably well. Also, a six-step ethylene reduced kinetic model is implemented in LES code to predict flame stability at the cavity flameholder experimental conditions.

## I. Introduction

Currently, hydrogen-fueled propulsion is preferred for hypersonic air-breathing engines with flight Mach numbers 10 or greater, due to the rapid burning and high mass-specific energy content of hydrogen. Hydrocarbon fuels become viable alternatives to hydrogen at Mach numbers below 10, because of their greater fuel densities and endothermic cooling capabilities [1]. However, hydrocarbon fuels pose an inherent difficulty for flame holding under high speed supersonic flows due to their long ignition delay times and shorter stability window for blow-off relative to hydrogen. In addition, changes in the chemical composition of fuel, which occur during endothermic cooling via thermal-catalytic reforming [2], will have an impact on fuel injection, mixing and flame-stability. Thus, one of the paramount difficulties in reactive flow simulation, both subsonic and supersonic conditions, is the development of a reduced kinetic model which is capable of predicting non-equilibrium, transient kinetic processes such as ignition and blow-out. Thus, in the present study, a new strategy for reduced kinetic model development is employed to simulate supersonic combustion of hydrocarbon fuels. Ethylene is chosen as the prototype fuel to develop and implement the reduced kinetic model to predict supersonic combustion phenomenon of a typical hydrocarbon fuel. Ethylene is also one of the common fuels studied experimentally under supersonic conditions due to its shorter ignition delay time compared to other hydrocarbon fuels. Rasmussen et al. [3] have performed experiments under supersonic conditions in a scramjet test facility to study ethylene stability phenomenon using cavity flame holders [4]. As the combustion stability under supersonic conditions is largely influenced by the interaction between the chemical kinetics and the turbulence transports, the experimental data reported by Rasmussen et al. [3] are used in the present study to validate the reduced kinetic models by implementing them in CFD code to simulate the cavity flame holder. Selected experimental conditions of Rasmussen et al. [3] for

<sup>1</sup> Senior Engineer, CSE, Inc., 8940 Old Annapolis Road, Suite L, Columbia, MD 21045, AIAA Member

<sup>2</sup> Project Engineer, CSE, Inc., 8940 Old Annapolis Road, Suite L, Columbia, MD 21045.

<sup>3</sup> Principal Engineer, CSE, Inc., 8940 Old Annapolis Road, Suite L, Columbia, MD 21045, AIAA Member

<sup>4</sup> Principal Engineer, CSE, Inc., 8940 Old Annapolis Road, Suite L, Columbia, MD 21045

<sup>5</sup> Technical Director, CSE, Inc., 8940 Old Annapolis Road, Suite L, Columbia, MD 21045, AIAA Member

<sup>6</sup> Graduate Student, School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, Student Member

<sup>7</sup> Professor, School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, AIAA Associate Fellow

rectangular cavity flame holder is simulated by implementing the ethylene reduced kinetic model in RANS and LES-LEM [5] codes to predict stable and blowout conditions.

## II Modeling Approach

As the operating envelope of flame-holding is confined by the boundaries of ignition, blow-out and flashback, the reduced kinetic models must be able to predict all three phenomena in order to predict the flame-holding. In addition, the kinetic models should be able to predict over a wide range of operating conditions considering the system fluctuations at the boundaries of flame-holding. The primary intermediate combustion radicals such as O, H, OH, HO<sub>2</sub> and H<sub>2</sub>O<sub>2</sub> play a major role in the transient, non-equilibrium processes, such as ignition and extinction, under high speed supersonic conditions. Therefore, a reduced kinetic model is developed in which a detailed kinetic model is included for CH<sub>2</sub>O/O<sub>2</sub> reaction scheme, which consists of the fundamental building blocks of any hydrocarbon oxidation. The H<sub>2</sub>/O<sub>2</sub> is followed by CO and CH<sub>2</sub>O reaction subset at the bottom of the hierarchical structure of a hydrocarbon oxidation mechanism. Thus, in the present approach, a detailed CH<sub>2</sub>O/O<sub>2</sub> reaction subset is included in the reduced kinetic mechanism such that it included detailed kinetic mechanism for H<sub>2</sub>/O<sub>2</sub> and CO/O<sub>2</sub> reaction sub-sets. For ethylene fuel decomposition, a single global reaction step is included in the reduced model. The reduced model consists of 14 species, namely, C<sub>2</sub>H<sub>4</sub>, CH<sub>2</sub>O, H<sub>2</sub>, H<sub>2</sub>O<sub>2</sub>, HO<sub>2</sub>, O, OH, H, HCO, CO, CO<sub>2</sub>, H<sub>2</sub>O, O<sub>2</sub> and N<sub>2</sub>. The fuel decomposition step is expressed as:



The rate of reaction,  $r$ , is expressed by a non-Arrhenius equation:

$$r = \left\{ AT^n e^{\left(\frac{-E}{RT}\right)} \right\} [\text{C}_2\text{H}_4]^{1.0} [\text{O}_2]^{1.0} \quad (2)$$

where A, E and n are the pre-exponential factor, activation energy and power dependence of temperature in non-Arrhenius rate constant, respectively. [C<sub>2</sub>H<sub>4</sub>] and [O<sub>2</sub>] refer to concentration of respective species. The estimated rate coefficients of the global reaction (1) is validated and optimized against shock tube ignition delay time measurements reported in the literature [6–12]. The conditions corresponding to the data used for the model validation are listed in Table 1. Due to experimental constraints, the experiments were performed using diluted mixtures of C<sub>2</sub>H<sub>4</sub>/O<sub>2</sub> in Ar with varying concentrations of C<sub>2</sub>H<sub>4</sub>.

Case #	Reference	Equiv. Ratio	Pressure	C <sub>2</sub> H <sub>4</sub>	O <sub>2</sub>	Ar
			(atm)	mole%	mole%	mole%
1	Kalitan et al. (2004) [7]	1.0	1	0.5	1.5	98.0
2	Horning (2001) [8]	1.0	1	1.0	3.0	96.0
3	Horning (2001) [8]	1.0	1	2.0	6.0	92.0
4	Horning (2001) [8]	1.0	1	4.0	12.0	84.0
5	Kalitan et al. (2004) [7]	1.0	3	1.0	3.0	96.0
6	Colket & Spadaccini (2001) [6]	1.0	7	0.7	2.1	97.2
7	Colket & Spadaccini (2001) [6]	0.5	6	0.7	4.2	95.1

Table 1: Experimental conditions for the shock tube ignition delay time measurements used to validate the ethylene reduced kinetic model.

The reaction rate coefficients for the fuel decomposition step are estimated by calibrating the ignition delay time model predictions against the shock-tube ignition delay time measurements of ethylene available in the literature. Optimized rate coefficients for the fuel-decomposition reaction are obtained by validating the reduced kinetic model against over a wide range of ethylene ignition delay time and flame-speed measurements available in the literature. Then, the reduced kinetic model is implemented in Star\*CD/KINetics to simulate supersonic experimental conditions of Rasmussen et al. [3], who performed a series of experiments in cavity flame- holder to study lean and rich blow-out limits of ethylene at Mach 2. Figure 1 shows the geometry of the rectangular cavity flame holder used for the experiments [3], and Table 1 shows the experimental conditions identified at stable, lean blowout and rich blowout.

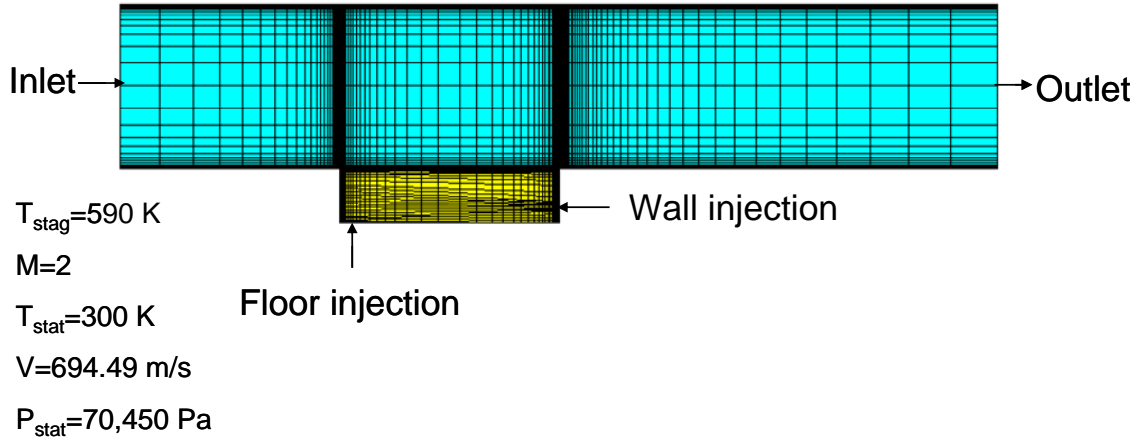


Figure 1: Grid geometry of a rectangular cavity-flame holder used supersonic experiments by Rasmussen et al. [3]. The CFD simulation was performed for two fuel injection positions as indicated. The length to depth ratio (L/D) of the cavity is 4.0.

Fuel Injection Point	Combustion Stability	Fuel Flow Rate - g/s
Wall	stable	1.6
	lean blowout	0.8
	rich blowout	4.7
Floor	stable	1.9
	lean blowout	0.6
	rich blowout	4.7

Table 2: Fuel flow rates measured experimentally [3] at stable, lean blowout and rich blowout at two different fuel injection points indicated in Figure 1.

### III RESULTS AND DISCUSSION

#### (a) Reduced Kinetic Model Development

Generally, the ignition delay time is defined as the time delay between the arrival of the reflected shock wave and the rise in pressure caused by the ignition. Another measure of the ignition-delay time is the time difference between the arrival of reflected shock wave and the emission from electronically excited OH\* or CH\* radicals formed during the induction period. When the initial reactant mixtures are diluted, the pressure rise is difficult to detect and hence introduce significant experimental error in the ignition delay time measurements [6]. Hence, the ignition delay time measurements selected for the model validation, listed in Table 1, were obtained by excited OH\* or CH\* emissions. The estimated rate constant in Eq. (2), which is validated and optimized against the ignition delay time measurements corresponding to the experimental conditions listed in Table 1 is, in cgs units:

$$k_1 = 5 \times 10^5 T^2 e^{\left(\frac{-10,000}{RT}\right)} \quad (3)$$

Figures 2 to 5 compare the ignition delay time predictions of the present reduced model with the shock tube experimental measurements. Also, the experimental measurements are compared with the ignition delay time predictions from two detailed mechanisms: an improved version of the detailed ethylene mechanism of Varatharajan and Williams [13] (denoted as UCSD Mech) and the GRI mechanism [14]. The GRI mechanism for natural-gas includes a detailed ethylene sub-mechanism as ethylene is one of the main intermediate of any hydrocarbon oxidation. Figure 2 compares the ignition delay time measurements of Kalitan et al. [7] performed at 1 atm with diluted mixtures of C<sub>2</sub>H<sub>4</sub>/O<sub>2</sub> in Ar. The reduced kinetic model and the detailed mechanisms predict the ignition delay time very well. Figure 3 compares the ignition delay time measurements of Horning [8] for three different mixtures (i.e., Case #2 through #4 in Table 1) with the model predictions. The CSE reduced mechanism predicts the ignition delay time for Case #2 and #3 very well compared to the detailed mechanisms. However, the CSE reduced model under-predicts the ignition delay time for Case #4 which has a low dilution reactant mixture compared to Case #1, #2 and #3. On the other hand, the detailed ethylene mechanism of Varatharajan and Williams [13] consistently under-predicts the ignition delay time for all of the cases.

Figure 4 compares the ignition delay of Kalitan et al. [7] for diluted, stoichiometric C<sub>2</sub>H<sub>4</sub>/O<sub>2</sub> mixture in Ar obtained at 3 atm pressure. Overall the reduced model and the detailed mechanisms predict the ignition delay time very well. It can also be observed that the models under-predict the ignition delay time at low temperatures. However, the detailed kinetic mechanisms over-predict the ignition delay time in the low-temperature region at high pressures as shown in Figure 5. Figure 5 compares the ignition delay time measurements of Colket and Spadaccini [6] with model predictions at 6 and 7 atm pressures. The reduced mechanism predicts the ignition delay time fairly well at these pressures over the entire temperature range. The poor prediction at low-temperatures by the detailed models is due to the fact that the increase in pressure shifts the low-temperature kinetics towards higher temperatures [15]. Thus, lack of low-temperature model validation of the detailed mechanisms caused the model predictions to be substantially different from the experimental measurements at low temperatures and high pressures.

Figure 6 shows the laminar flame speed predictions of C<sub>2</sub>H<sub>4</sub>/air mixtures at 1 atm compared with the experimental measurements of Egolfopoulos et al. [16]. It can be noted that the ethylene reduced model predicts the laminar flame speed reasonably well up to an equivalence ratio of 1.5. The detailed ethylene mechanism of Varatharajan and Williams [13] predicts the experimental data very well, while the GRI mechanism consistently over-predicts the flame speed.

Overall, the reduced kinetic mechanism developed in the present work predicts the ignition delay time and laminar flame speed measurements of ethylene reasonably well. The reduced kinetic mechanism showed a superior predictive capability for ignition delay time compared to detailed ethylene mechanism as demonstrated above.

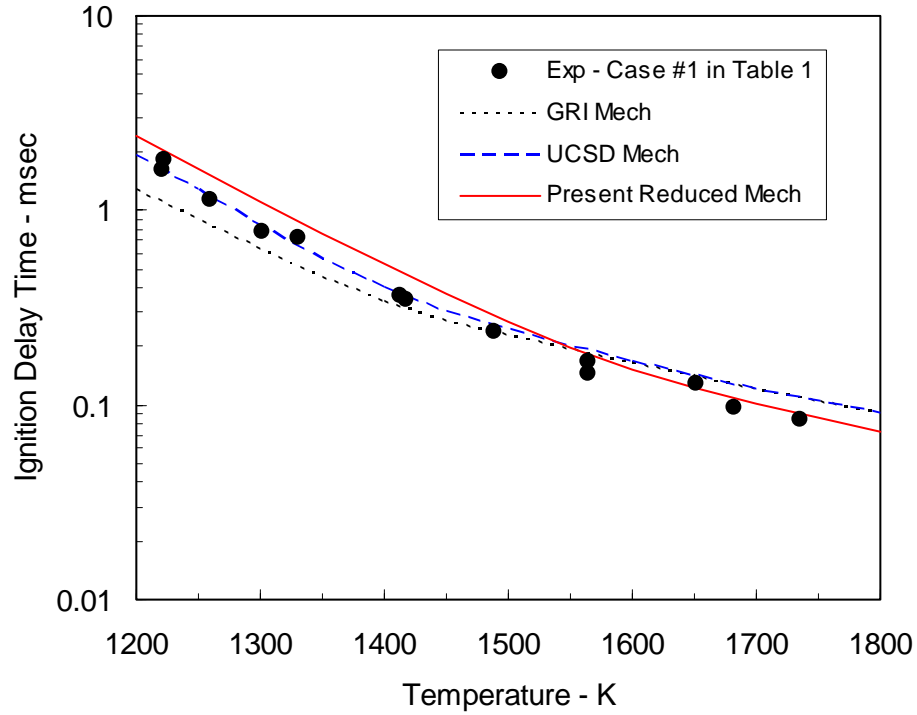


Figure 2: Shock tube ignition delay time measurements of Kalitan et al. [7] (i. e, Case #1 in Table 1) are compared with model predictions. Key: symbols denote experimental data and lines denote model predictions. Solid line – present reduced kinetic mechanism; dotted line – GRI3.0 mechanism [14]; dashed line – UCSD mechanism [13].

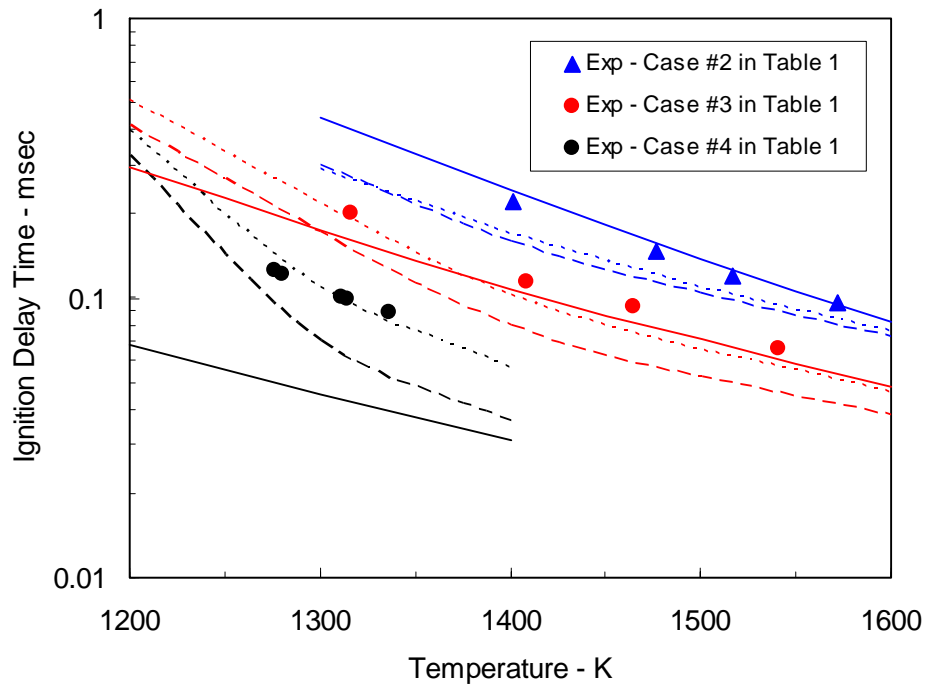


Figure 3: Shock tube ignition delay time measurements of Horning [8] (i. e, Case #2 to #4 in Table 1) are compared with model predictions. Key: symbols denote experimental data and lines denote model predictions. Key: as in Figure 2.

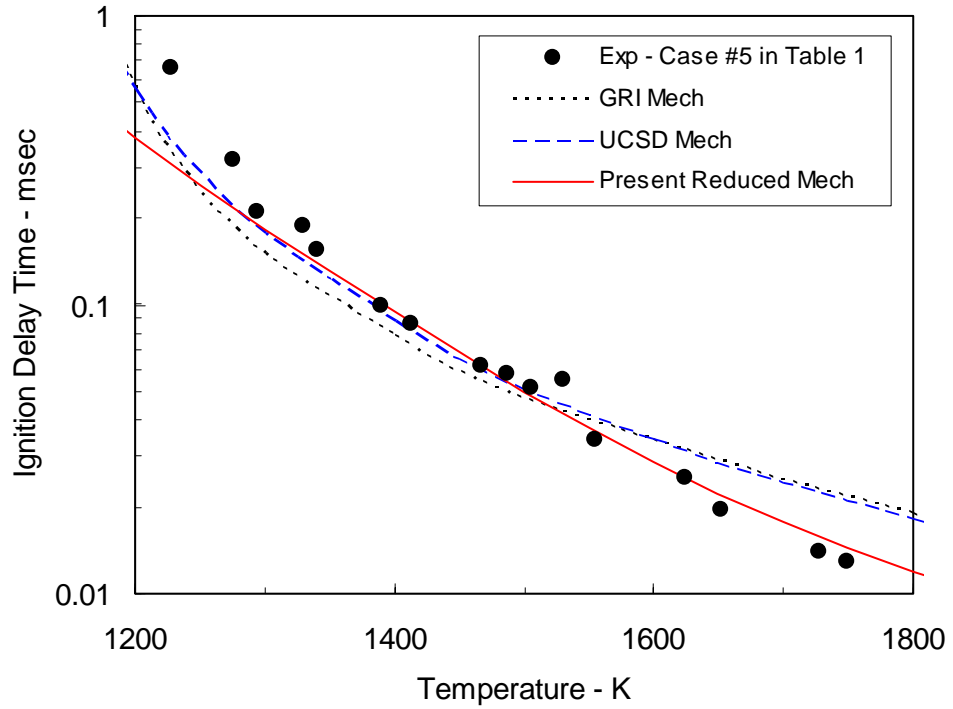


Figure 4: Shock tube ignition delay time measurements of Kalitan [7] (i. e., Case #5 in Table 1) are compared with model predictions. Key: same as in Figure 2.

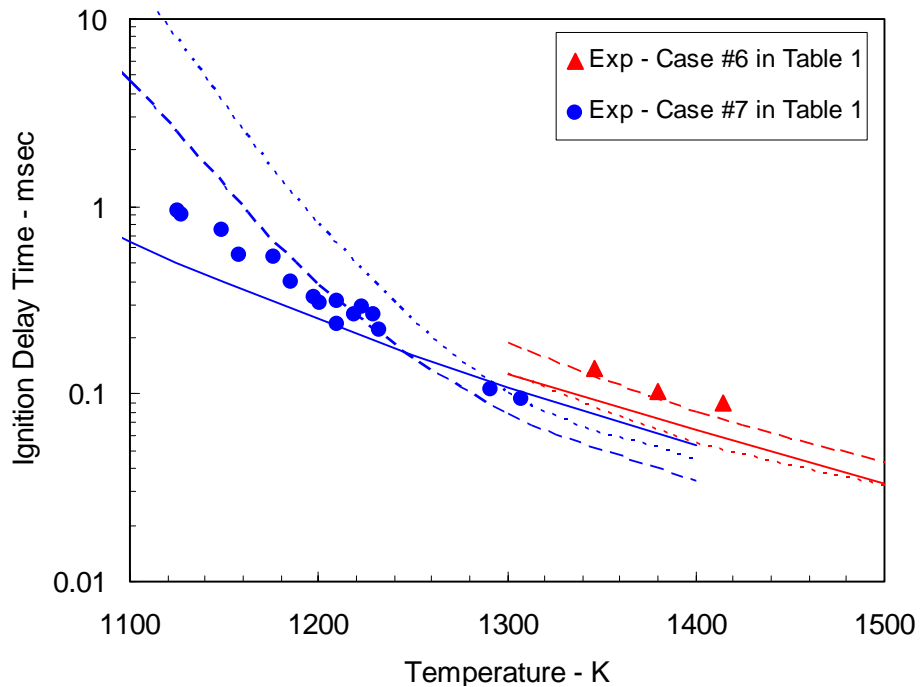


Figure 5: Shock tube ignition delay time measurements of Colket & Spadaccini [6] (i. e., Case #6 and #7 in Table 1) are compared with model predictions. Key: same as in Figure 2.

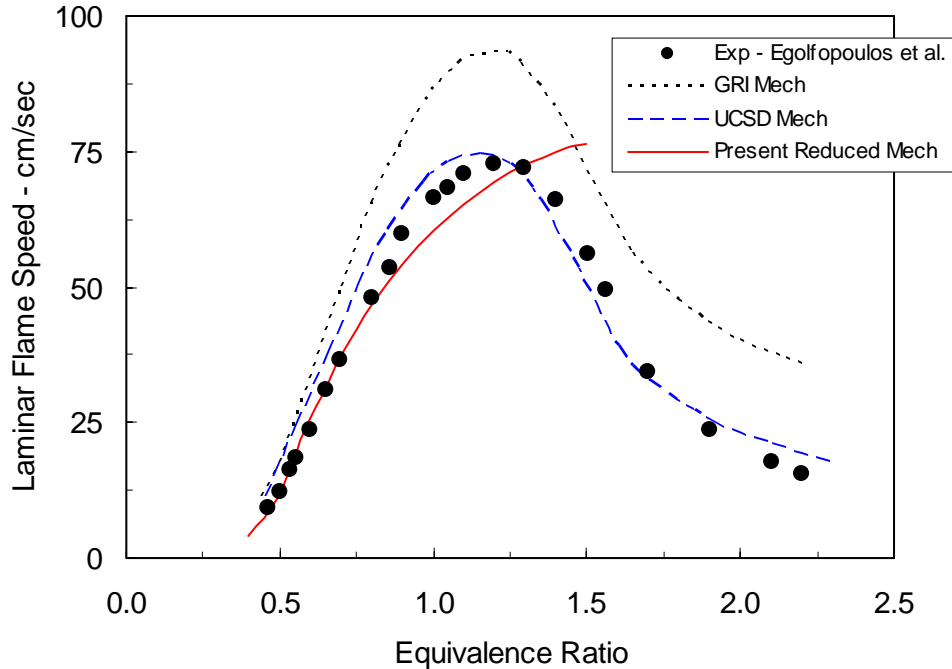


Figure 6: Laminar flame speed measurements of Egolfopoulos et al. [16] are compared with CSE reduced model as well as detailed ethylene mechanism [13] and GRI mechanism [14] as indicated.

### (b) Model Implementation in CFD Code

The ethylene reduced kinetic model developed above was implemented in Star\*CD/KINetics [17] to simulate the rectangular cavity flame-holder shown in Figure 1 for the experimental conditions specified in Table 2. The cavity temperature profile obtained in the RANS simulation is used to identify the stable and blow-out conditions. Figure 7 shows the cavity temperature profile at stable conditions observed experimentally by Rasmussen et al. [3] at wall injection, i.e. with 1.6 g/s fuel flow rate in Table 2. It can be noted that the flame occupies the cavity with maximum temperature of 2400 K. Figure 8 demonstrates the lean blowout predictions of the reduced model as observed experimentally by Rasmussen et al. [3] with fuel flow rate of 0.9 g/s. As noted in Table 2, lean blowout was experimentally observed at 0.8 g/s fuel flow rate [3]. Thus, the reduced kinetic model predicts the stable and lean blowout conditions reasonably well. Figure 9 shows the CFD simulation when the fuel flow rate was 5 g/s. Figure 10 depicts the average cavity flame temperature as a function of fuel flow rate for wall injection. It can be observed that there is sharp drop in temperature around 0.9 g/s fuel flow rate. This indicates the lean blowout fuel flow rate that was noted by Rasmussen et al. [3]. However, at fuel-rich condition, the temperature remains constant around 1300 K for fuel rates higher than 5 g/s. However, Rasmussen et al. [3] observed that the rich blow-out occurred at 4.7 g/s with difficulty in distinguishing stable and blowout at fuel rich conditions. The CFD simulations and experimental observation implies that reduced model predicts the rich blow-out around 5 g/s fuel flow rate. It appears that the temperature increase observed above 5 g/s fuel flow rate is due to the heat generated during fuel break caused by the isentropic temperature increase at high Mach numbers.

The implementation of the ethylene reduced kinetic mechanism in Star\*CD predicts the stable combustion and lean blow-out fairly well. To further investigate the chemistry-transport interactions under supersonic flow conditions, a six-step ethylene reduced kinetic model is implemented in LES code for stable combustion condition with a resolution of 261x80x27 in the main stream and 91x71x27 in the cavity. A single fuel injector located at the wall of the cavity is simulated with a mass flow-rate of 1.6 g/s. For this study, ethylene is injected at room temperature and at constant pressure. Ignition is triggered by initially increasing the temperature in the cavity, and eventually, the solution settles down. Figure 11 shows the instantaneous temperature profile. Figure 11 shows a highly unsteady behavior inside the cavity which can be captured by a time-dependent simulation technique. It appears that the flame and high temperatures are formed at the upstream side of the cavity with a maximum of around 2500K.

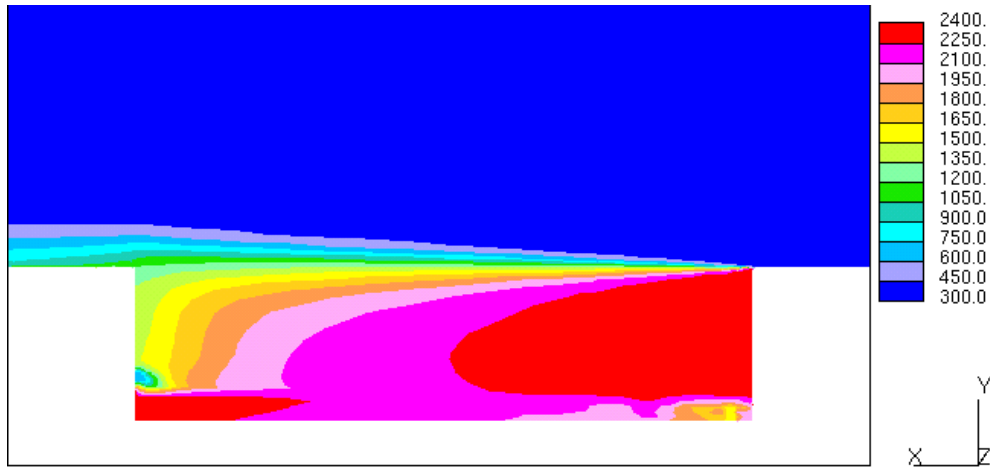


Figure 7: RANS simulation of rectangular cavity flame-holder shown in Figure 1 at stable combustion with 1.6 g/s fuel flow rate with wall injection.

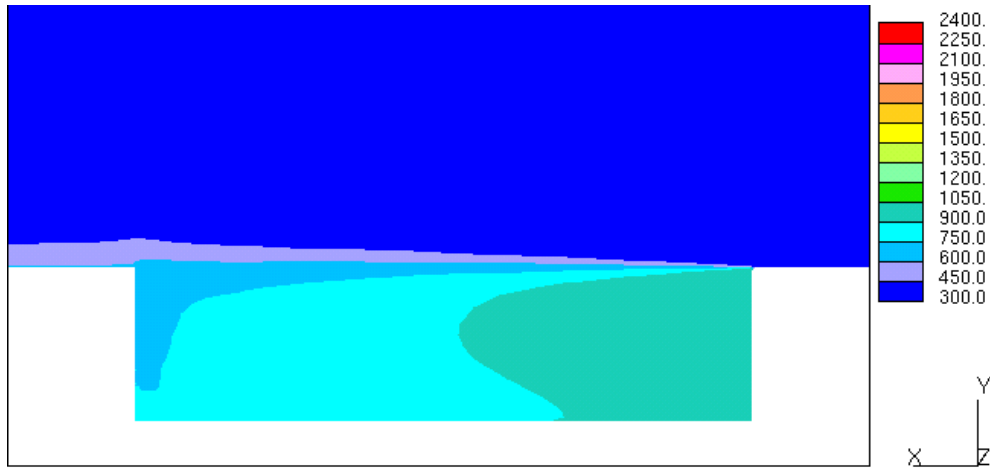


Figure 8: RANS simulation of rectangular cavity flame-holder shown in Figure 1 at lean blowout condition with 0.9 g/s fuel flow rate with wall injection.

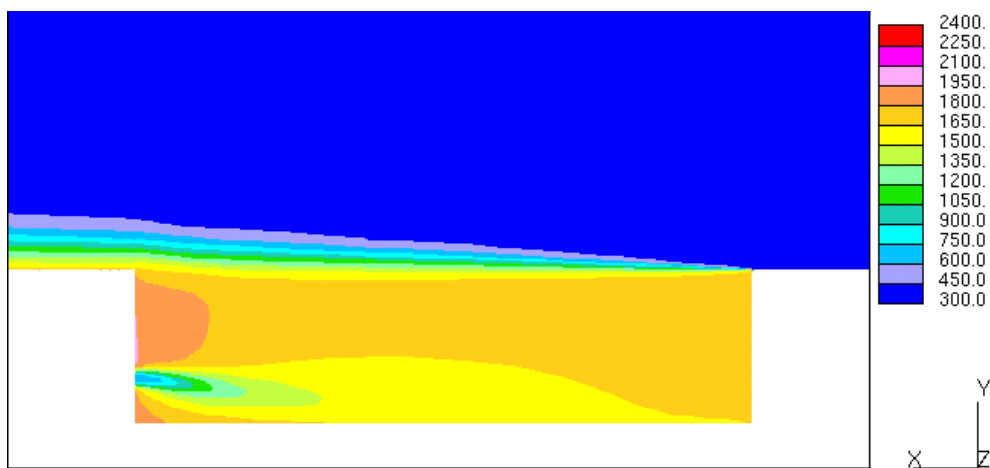


Figure 9: RANS simulation of rectangular cavity flame-holder shown in Figure 1 at rich blowout condition with 5.0 g/s fuel flow rate with wall injection.



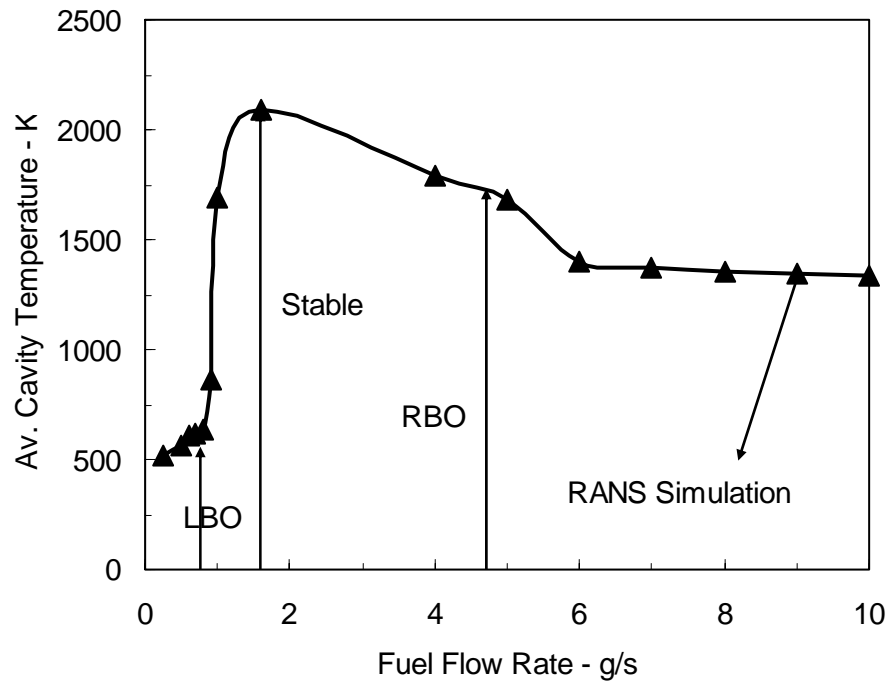


Figure 10: Average cavity temperature as a function of fuel flow rate obtained by implementing the ethylene reduced kinetic model in Star\*CD/KINetics for the experimental conditions specified in Figure 1 with fuel injection from the wall. LBO, RBO and stable refer to the fuel flow rates corresponding to lean blow-out, rich blow-out and stable conditions observed in Rasmussen et al. [3] cavity flameholder experiments, respectively.

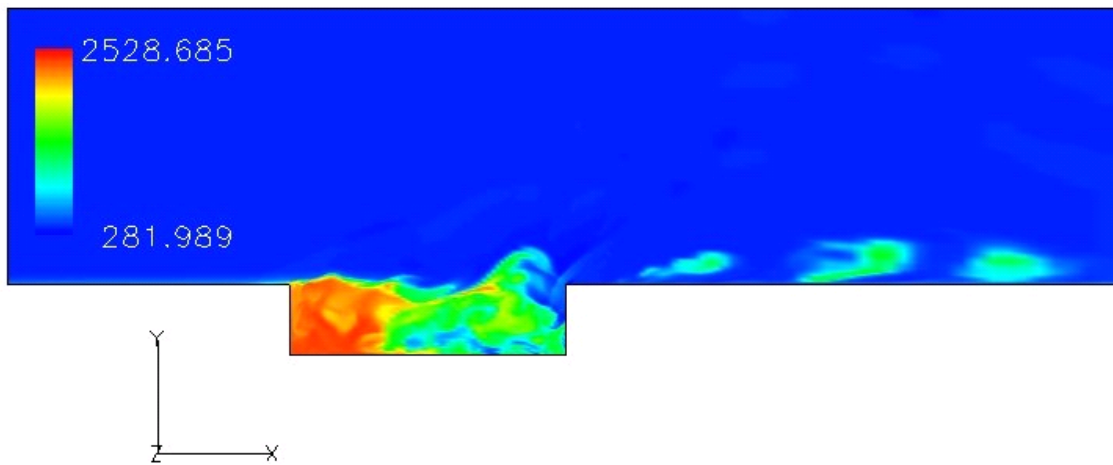


Figure 11: Instantaneous snapshot of the temperature contours in the symmetry plane generated by LES simulation of the rectangular cavity flame-holder shown in Figure 1 at stable combustion with 1.6 g/s fuel flow rate with wall injection.

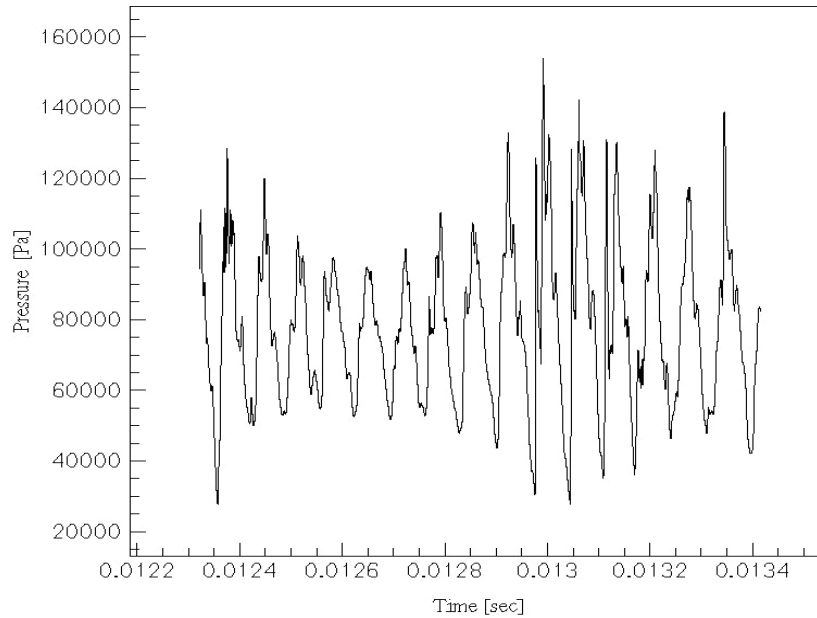


Figure 12: A time trace of pressure oscillations in the cavity for the conditions shown in Figure 11

Figure 12 shows the pressure oscillations inside the cavity that can affect the injection of fuel into the cavity. Since the fuel is supplied at a constant pressure, the oscillation inside the cavity changes the mixing characteristics of fuel and this effect is captured by the LES approach.

#### IV Conclusion

The primary goal of this project is to develop a general purpose design tool to generate reduced kinetic mechanisms of hydrocarbon fuels which can be incorporated into CFD codes to simulate scramjet combustion systems during the design process. The feasibility of the reduced kinetic modeling strategy proposed by CSE to simulate supersonic flow conditions was successfully demonstrated in Phase I. Reduced kinetic models were developed for ethylene and Jet-A fuels. Reduced kinetic models were validated and optimized against ignition delay time data and laminar flame speeds. Ethylene was used as a prototype fuel to demonstrate this strategy by implementing the ethylene reduced kinetic model in RANS and LES CFD codes to simulate cavity flame holder experiments. The ethylene reduced kinetic model was able to predict the stable and blow-out conditions reasonably well.

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