# Three-Dimensional Simulation of Turbulent Hot-Jet Ignition for Air-$CH_4$-$H_2$ Deflagration in a Confined Volume

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## Abstract

This work describes essential aspects of the ignition and deflagration process initiated by the injection of a hot transient gas jet into a narrowly confined volume containing air-$CH_4$-$H_2$ mixture. Driven by the pressure difference between a pre-chamber and a long narrow constant-volume-combustion (CVC) chamber, the developing jet or puff involves complex processes of turbulent jet penetration and evolution of multi-scale vortices in the shear layer, jet tip, and adjacent confined spaces. The CVC chamber contains stoichiometric mixtures of air with gaseous fuel initially at atmospheric conditions. Fuel reactivity is varied using two different $CH_4$/$H_2$ blends. Jet momentum is varied using different pre-chamber pressures at jet initiation. The jet initiation and the subsequent ignition events generate pressure waves that interact with the mixing region and the propagating flame, depositing baroclinic vorticity. Transient three-dimensional flow simulations with detailed chemical kinetics are used to model CVC mixture ignition. Pre-ignition gas properties are then examined to develop and verify criteria to predict ignition delay time using lower-cost non-reacting flow simulations for this particular case of study.

**Keywords:** Hot jet ignition, Constant volume combustor, Pre-chamber ignition

## 1. Introduction

Deflagration initiation by injection of hot gas into a fuel-air mixture is important in combustion engines, explosion protection and fire safety. Turbulent hot-jet ignition can be a reliable means of

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rapid ignition of fuel-lean mixtures in stratified internal-combustion (IC) engines and in wave rotor combustors (WRC) with high effectiveness [1]. Ignition by a turbulent jet was investigated in the 1950's by Noble-prize-winner Nikolai Semenov [2] and was further established by Gussak et al., [3] and Oppenheim [4] for IC engine applications, emphasizing the role of radicals from a chemical perspective. Jet hydrodynamics was studied by Oppenheim [2] and co-workers elaborating the factors by which jet penetration and dispersion could be controlled. The penetrative hot jet which normally contains chemically active radicals can act as a distributed source of ignition. The temporal and spatial evolution of the transient jet involves complex features as the walls interact acoustically and aerodynamically with the developing jet [5].

Prior work in relatively unconfined mixtures included attempts to correlate the jet characteristics such as temperature, momentum and orifice diameter to ignition success. The location of ignition by an inert, laminar hot jet was described by a simplistic plug flow reactor model backed by empirical data [6]. As expected, the ignition takes place closer to the nozzle as the jet temperature increases and farther away as the jet velocity increases. However, if turbulence enhances mixing, the effect of jet velocity on ignition may be more nuanced. Ignition success involves a competition and a collusion between chemical time scale and the mixing time scale of jet entrainment, diffusive transport, and mixing at smaller scales. The overall thermal-chemical balance determines whether the exothermic reactions prevail and ignition takes place. Imbalanced transport of heat and reactants may quench ignition. As the jet contains active radicals that are a product of a primary combustion in the pre-chamber, an appropriate model would consider this in achieving cost-effective predictions of ignition.

The critical minimum radius for the jet (under which ignition is suppressed) is evaluated and prescribed to be necessarily larger than the deflagration thickness of the flame [7]. Subsequently, for a given injection velocity the smallest critical radius is found at stoichiometric mixture [8, 9]. The impact of jet momentum on turbulent jet ignition (TJI) has received various numerical

investigations in literature. Increasing the jet Reynolds number may prolong ignition delay [9]. In a 2D simulation of TJI of $H_2$-air, increasing the jet velocity and thus the turbulence intensity in the shear layer may suppress ignition due to excessive cooling [10]. By tracking the jet tip, ignition was sometimes observed at the jet crown where stream impingement strongly promotes mixing [10]. However, the ignition core may be transported towards the lateral face of the jet as the tip advances within the cold environment [11, 12]. Through a comparative assessment of literature, the authors of present work speculate about the effect of Damkohler number on the probability of ignition at the vortex or shear layer of trailing jet.

In contrast with typical IC engine geometry, the long and narrow CVC considered in the present work is typical of a wave-rotor combustion channel, with length/width aspect ratio of the order of 10, and chamber width only about 5 times the jet nozzle diameter. Upon jet entrance, and more so after ignition, a series of pressure and expansion waves propagate in the CVC and interact with the jet and with the initiated flame through Richtmyer-Meshkov vorticity deposition, amplifying the local heat release rates [13]. The waves and the jet evolving within confining walls exhibit hydrodynamic behavior and form complex three-dimensional structures that can influence ignition. Prediction of ignition requires an accounting of jet or puff penetration and three-dimensional vortical structure evolution for the confined CVC geometry, with entrainment of fuel-air mixture. Prior numerical investigations in the literature of unconfined transient jets were often conducted using a 2D axisymmetric approach to save computational time. However, experimental observations show that even an unconfined turbulent hot jet has highly asymmetric behavior, with jet evolution and jet ignition being sensitive to small perturbation of symmetry. In a confined volume, flame propagation with wave interactions is also highly multi-dimensional. The present study employs transient 3D simulation to describe the underlying physics and chemistry of TJI in a confined volume containing $CH_4$-$H_2$ blend premixed with air. The study seeks an ignition probability criterion that can be used to predict the possibility of ignition development. Numerical approach

and validation are introduced in Section 2. In Section 3, ignition and flame propagation phenomena are studied in a numerical domain for a stationary pre-chamber. Based on the knowledge obtained in Section 3 and works of Khan [14], Section 4 is aimed at proposing ignition criterion that serves to predict the ignition event for the studied stationary jet and traversing jet configurations.

## 2. Problem Description and Numerical Methodology

One goal of the present study is to aid development of an experimental rig by the authors and co-workers, intended to replicate ignition in a WRC with ignition by transfer of hot gas between its channels. As shown in Fig. 1, a cylindrical rotatable pre-chamber is used to generate a jet of hot combustion products that is precisely injected into a long rectangular CVC chamber via a converging nozzle, to create a traversing hot jet similar to that in a WRC. The pre-chamber has an internal volume of approximately 0.835 L. The CVC chamber is 40.64 cm long and has a square cross section with 3.98 cm sides. The connecting nozzle (not visible) has 6 mm exit diameter, 10° taper and 25mm length.

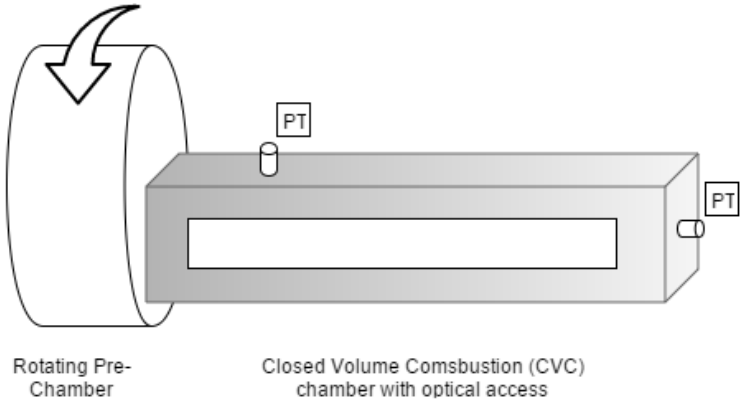


**Figure 1. Schematic of the hot-jet ignition rig**

In the experiment, the rotating pre-chamber contains fuel-air mixture and is ignited with a spark plug. The pressure of combustion eventually and predictably causes rupture of a carefully scored thin aluminum diaphragm separating the pre-chamber and CVC chamber, which also holds premixed air and fuel at slightly rich equivalence ratio. The diaphragm rupture is triggered to

exactly precede traverse of one end of the CVC by the nozzle, allowing a high-speed jet of combustion products to be injected into the CVC. For the simplicity of the simulation, the pre-chamber is assumed to be filled with combustion products at equilibrium temperature and composition prior to the rupture moment. The current work focuses on the effect of two main operating conditions which are the pre-chamber pressure and the fuel reactivity in the CVC on the ignition properties and flame propagation. In the experiment, the pressure of the pre-chamber at the rupture moment can be controlled by the diaphragm scoring technique [15]. In the simulations, the pressure in pre-chamber is set as an initial condition. The fuel reactivity in the CVC is represented by different blend ratios of $CH_4$ and $H_2$.

In order to develop better insight into jet ignition and subsequent flame propagation, a set of simulations for stationary pre-chamber are conducted at which the injection pressure and fuel blends are varied, while the jet nozzle is fixed at the CVC axial centerline. The list of studied cases is provided in Table 1.

**Table 1. Case studied for stationary pre-chamber pressure and CVC chamber fuel blends**

| Case Number | Pre-chamber Pressure (bar) | CVC fuel blends (by volume) |
|---|---|---|
| 1 | 2 | Fuel-LR, 50:50 $CH_4 - H_2$ |
| 2 | | Fuel-HR, 30:70 $CH_4 - H_2$ |
| 3 | 4 | Fuel-LR, 50:50 $CH_4 - H_2$ |
| 4 | | Fuel-HR, 30:70 $CH_4 - H_2$ |
| 5 | 6 | Fuel-LR, 50:50 $CH_4 - H_2$ |
| 6 | | Fuel-HR, 30:70 $CH_4 - H_2$ |

For brevity, the higher reactive 30:70 $CH_4$-$H_2$ blend will be called `Fuel-HR' and the lower reactive 50:50 $CH_4$-$H_2$ blend will be called `Fuel-LR' throughout this study. The mass of each fuel blend is calculated so that the total chemical energy is almost equal in all the cases. The reactivity level of

the blends is judged based on their ignition delay in a shock tube experiment [16]. Kinetic simulations done by the authors using Cantera® [17] show that on average Fuel-HR has shorter chemical autoignition delay by 76% comparing to the Fuel-LR within the temperature range of 1100-1900K at 1 bar.

Preliminary experiments suggest that slightly rich combustion in the pre-chamber provides the most rapid and consistent ignition, given ambient room conditions of pre-chamber initial mixture, for a wide range of CVC conditions [14, 18]. Therefore, the equilibrium temperature, pressure, and composition of the pre-chamber at equivalence ratio of 1.1 is calculated and applied to all the cases for initializing the simulation [18, 19]. The initial thermal and chemical properties of pre-chamber and CVC chamber are listed in Table 2.

**Table 2. Initial temperature, equivalence ratio and mass fraction**

| **Thermodynamic properties** | **Pre-chamber** | **CVC chamber Fuel-LR** | **CVC chamber Fuel-HR** |
|---|---|---|---|
| Equivalence ratio | 1.1 | 1 | 1 |
| Temperature(K) | 2670 | 300 | 300 |
| Pressure (atm) | 2, 4 ,6 | 1 | 1 |
| $Y_{N2}$ | 0.72364 | 0.72872 | 0.73211 |
| $Y_{O2}$ | 0.0026 | 0.22144 | 0.22252 |
| $Y_{H2}$ | 0.00137 | 0.00553 | 0.01023 |
| $Y_{CH4}$ | 0 | 0.04431 | 0.03514 |
| $Y_{OH}$ | 0.0038 | 0 | 0 |
| $Y_{O}$ | 0.00026 | 0 | 0 |
| $Y_{H2O}$ | 0.14883 | 0 | 0 |
| $Y_{H}$ | 0.0000786 | 0 | 0 |

| | | | |
|---|---|---|---|
| $Y_{CO2}$ | 0.08641 | 0 | 0 |
| $Y_{CO}$ | 0.02991 | 0 | 0 |
| $Y_{NO}$ | 0.0031 | 0 | 0 |

For the simulation of the reacting turbulent transient flow, the CONVERGE code is used [20]. Turbulence is modeled using two-equation k-ε RNG model, [21] and chemistry is modeled using the code's detailed kinetics solver, called SAGE. The reduced reaction mechanism DRM19 is used [22], which consists of 19 reactive species (plus $N_2$ and Ar) and 84 elementary chemical reactions, with associated thermochemical properties. In comparison with the more detailed GRI 3.0 mechanism for natural gas [23], the DRM19 mechanism showed 6-8 % deviation for ignition delay times and laminar flame speeds of mixtures at equivalence ratio of 0.2-2.0, initial pressure of 0.1-50 atm, and initial temperature of 1000-2500 K [24]. Even when employed beyond the expected temperature range of validity, GRI based mechanisms showed the best agreement with experimental measurements of jet ignition experiment [25, 26, 27]. However, the fact must be noticed that unlike the standard ignition studies, the jet ignition produces fuel and oxidizer kernels that are highly contaminated by the active radicals generated in the pre-chamber. Therefore, the initiation elemental reaction rates are augmented which might extend the applicability of detailed mechanisms in terms of temperature. For more efficient computation, the SAGE solver uses multi-zone modeling, grouping cells in zones based on their thermodynamic state, with each zone treated as a closed-volume homogeneous reactor. In the current study, a three-variable multi-zone approach is employed which uses temperature, total equivalence ratio, and methane concentration to establish the zones with similar properties.

Employing adaptive mesh refinement (AMR), the cell size distribution is chosen to provide adequate resolution for turbulent flame fronts and reasonably sharp representation for pressure waves to model acoustic interactions. Using a preliminary estimation of viable ignition kernel size

based on William's ignition criterion [28] to be about 0.1 mm, the mesh refinement is adjusted to place 8 to 10 computational cells in ignition initiation regions to ensure adequate resolution for ignition detection and ability to resolve the flame thickness. A total cell count as high as 10 million was reached as the cell size was adaptively refined to uniformly resolve temperature and velocity gradients. Figure 2 shows the numerical domain and refined grid utilized for the simulations. In the current work, a second-order accurate spatial discretization scheme and a fully implicit first-order accurate time-integration scheme are used to solve the governing conservation equations. A variable time scale algorithm is used, with time-step varied between $10^{-8}$ and $10^{-5}$ seconds. The transport equations are solved using the pressure-implicit-with-splitting-of-operators (PISO) method of Issa [29]. The time-step is automatically maximized for stability in each computational cycle based on velocity and local speed of sound. The computational facility used in this study is a 64-node sector of Indiana University's BIG RED II supercomputer where each node contains two AMD Opteron 16-core x86_64 CPUs and 64 GB of RAM.

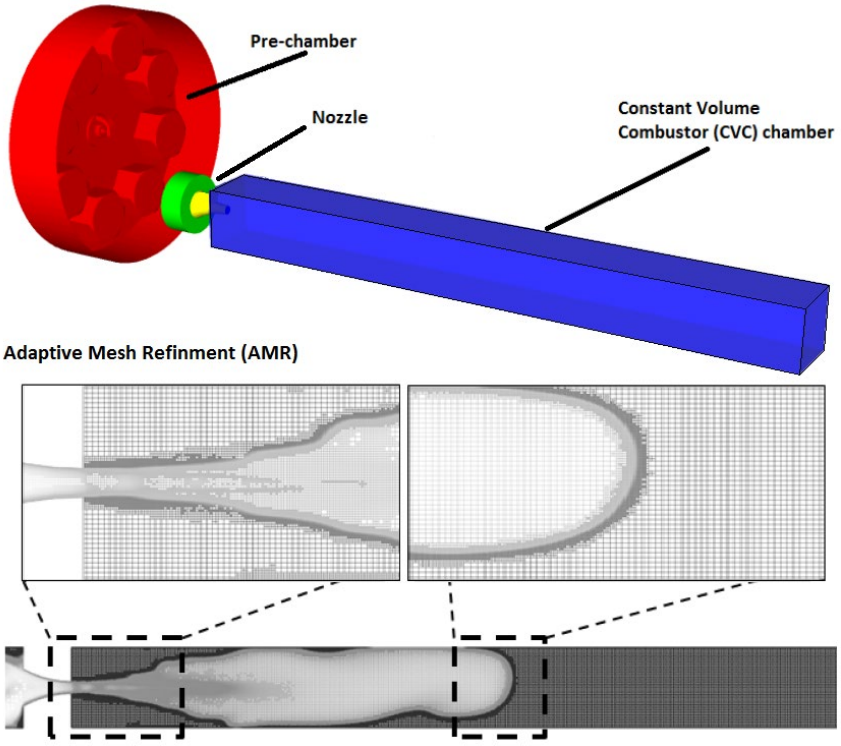


**Figure 2. The 3D numerical domain and local mesh refinement employed**

## 3. Characteristics of Ignition

### 3.1. Validation with PFR analysis

To validate aspects of the approach, representative numerical simulations are first compared with another recognized study. The ignition location obtained by the simulations are compared with the semi-empirical model developed by Fink and Vanpee [6] which employs plug-flow reactor (PFR) analysis to make a correlation between jet velocity, ignition distance, and rate constants of the global reaction rate. The simplistic model assumes that mixing of the hot jet and CVC mixture happens much faster than the chemical time scale and also that ignition occurs closer to the hot jet rather than the cold mixture with respect to the mixing shear layer. Therefore, the process is modeled as a PFR in which a portion of fuel and oxygen is diluted in a batch of active hot gas, and the chemical kinetic process begins. The mixture would ignite after undergoing conversion during a contact time, $\frac{z}{U_{cl}}$ which can be formulated as:

$$\frac{z}{U_{cl}} = \int_{Y_i^O}^{Y_i^F} (M_i \, \rho \, dY_i)/W_i \qquad (1)$$

Where $U_{cl}$ and $z$ are jet velocity at the nozzle centerline and ignition distance from the nozzle, respectively. The reaction rate $W_i$ used in Eq. 1, for the fuel is of the form:

$$W_f = A \, M_f \, e^{-\frac{E}{RT}} \left(\frac{P}{RT}\right)^{C+D} Y_f^C \, Y_O^D \qquad (2)$$

where $A$ and $M_f$ are pre-exponential constant and fuel molecular weight, respectively. Substituting the rate reaction of Eq. 2 into the integral and applying the logarithm to both sides, the integral yields;

$$\log\left(\frac{U_{cl}}{z}\right) = -\frac{E}{RT} + \log\left(\frac{Y_F^C Y_O^D A}{Y_O - Y_F}\right) - (C + D - 1)\log(T/P) \qquad (3)$$

$T$, $P$ and $R$ are jet temperature, CVC pressure and gas constant, respectively. $E$ is the activation energy and $C+D$ is total order of reaction. According to Eq. 3, for a given fuel mixture, the quantity $\log\left(\frac{U_{cl}}{z}\right) + (C + D - 1)\log(RT/P)$ vs. $\frac{1}{T}$ should generate a linear plot with a slope of $-\frac{E}{R}$. It is implied by Eq. 3 that if the jet temperature and fuel-air composition of the CVC are kept constant, the variation of ignition distance with respect to the jet velocity should adjust itself in a fashion that $\log\left(\frac{U_{cl}}{z}\right)$ remains nearly constant.

Table 3 displays the left-hand side value of Eq. 3, $\log\left(\frac{U_{cl}}{z}\right)$, for different jet momentum (pre-chamber pressures) along with the corresponding jet velocities and ignition distances. The jet velocity is read on the centerline one diameter downstream of the nozzle tip and the ignition distance is identified by the abrupt rise of OH concentration in the spatial field. For the present cases of study, $E$ is assumed to be equal to 37.79 kcal/mol based on the study of Zhang et al. [16] that examined the ignition delay of $H_2$-$CH_4$ blends in the shock tube experiment. The order of global reaction with respect to the tri-component reactant is known to be 1.1[6]. This value is developed by establishing a relation between rate of global reaction and laminar speed of the flamelets. As expected by Eq. 3, the value of $\log\left(\frac{U_{cl}}{z}\right)$ does not vary significantly by changing the pre-chamber pressure which controls the jet momentum. This behavior is consistent with the observations of Sangras et al. [30], which showed the self-preserving properties of developing turbulent jets in a still environment.

**Table 3. Verifying the self-preserving development of the hot jet ignition**

Jet Temperature:2670 K, CVC Fuel-HR

| **Pre-chamber pressure (bar)** | **U (m/s)** | **z (cm)** | $\log\left(\frac{U_{cl}}{z}\right)$ |
|---|---|---|---|
| 2 | 700 | 8.4 | 3.92 |
| 4 | 860 | 13.1 | 3.81 |
| 6 | 1000 | 14.5 | 3.83 |

### 3.2. Comparison with literature

There are only a few experiments and numerical efforts reported on ignition by a hot jet in a confined volume that are closely similar to the present work. Two of the critical factors discussed in the literature which are known to strongly influence the jet ignition delay are orifice diameter and the fuel reactivity in the CVC. Mayinger et al. investigated the scalability of jet ignition devices by employing various orifice diameters and measuring the ignition delay [31]. It was shown that with orifice diameter of 6 mm, the reported ignition delay for propane-air mixture at the mixture equivalence ratio of 0.62 is below 2 ms. This result would agree with all of the findings of the present study that are done with a 6 mm nozzle size. In another similar study conducted by Ghorbani et al. [11] it is stated that for jet ignition of hydrogen-air mixture, the ignition delay varies in the range 0.1-0.4 ms, depending on the jet entrance temperature. In the present work, for the hydrogen-dominated mixtures (70%$H_2$-30%$CH_4$), the ignition delay is approximately 0.8 ms which reasonably agrees with Ghorbani's.

Preliminary experiments using the ignition rig modeled in Paik's study [15] examined the significance of jet momentum on the ignition delay of methane-hydrogen fuel blends. Figure 3 presents a comparison between the experimental and numerical measurements of ignition delay for similar fuel blends at standard condition. The trend of decreasing ignition delay with higher jet momentum is supported. The shorter predicted ignition delay likely stems from higher jet temperature comparing to the experiments. Based on ongoing (unpublished) infra-red imaging of the jet in the experimental rig, the jet temperature during discharge is lower than the pre-chamber temperature postulated in the present simulations, mainly due to unaccounted heat losses.

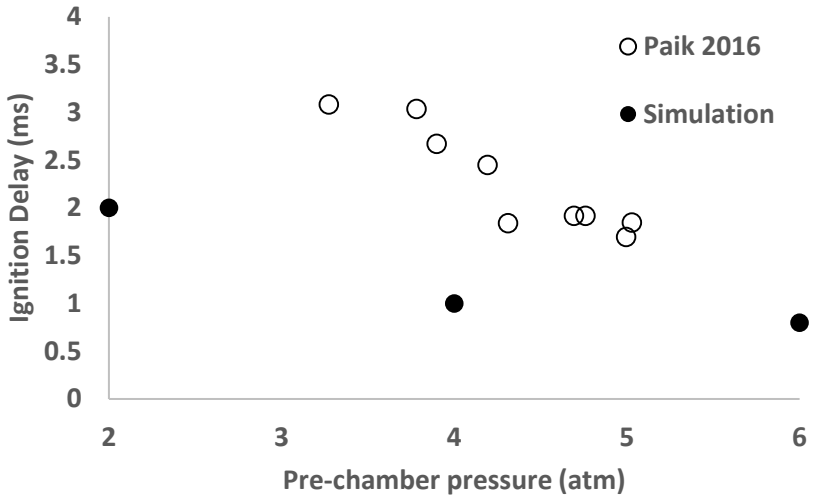


**Figure 3. Minimum ignition delay measurements for 70%$H_2$-30%$CH_4$ fuel blend**

### 3. 3. Effects of Pre-Chamber Pressure and CVC Chamber Fuel Reactivity

For ignition by a jet of reactive hot gas, there is a significant physical mixing process that must occur before chemical reactions can commence, yet the injected reactive species should ideally remain chemically active while the jet mixes with relatively cold reactive gas.

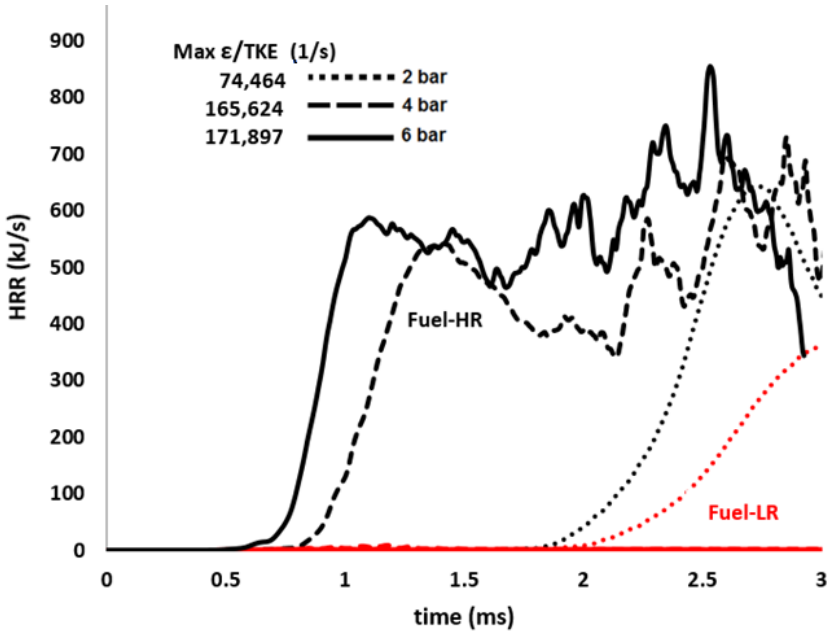


**Figure 4. History of heat release rate with varied fuel reactivity and jet momentum**

The ignition delay time for a jet-ignited CVC may be defined as the time from the emerging of the initial hot jet to the occurrence of rapid, visible, and pressure-generating heat release. The authors observed that ignition often occurs where fuel, air, and injected hot gas are mixing in small distinct regions that are within the critical ignition kernel size and are experiencing temperature above auto ignition conditions for that particular composition.

The instantaneous heat release rate (HRR) accompanied with the local OH production in the CVC chamber is used in this study to indicate the ignition delay. The computed history of the reaction heat release rate (J/sec) in the CVC chamber is presented in Fig. 4. The ignition event can be recognized by the sudden rise of HRR curve.

For Fuel-HR, Fig. 4 reveals the positive effect of increasing jet momentum on shortening the ignition delay. Also, all of the simulations for the Fuel-HR led to a successful ignition event whereas for Fuel-LR, the ignition only occurs for pre-chamber pressure of 2 bar, whereas for higher jet momentum, no significant reaction is initiated during the simulation time of 3 ms. The opposite effect of the jet momentum on the ignition delay for Fuel-HR compared to Fuel-LR is notable and needs to be addressed. As discussed earlier, the ignition success is decided by two processes acting in parallel: the hot jet providing the thermal energy and some radicals, and the heated reactant mixture undergoing initiation reactions leading up to ignition. If the chemical time scale ($\tau_{ch}$) which is inversely related to fuel reactivity is longer than the mixing time scale ($\tau_{mix}$), the batch of fuel-air containing hot gases might cool down due to excessive mixing with the cold environment before it can launch the ignition reactions.

The amount of turbulence induced by the high velocity jet plays a major role in mixing the two fluids. Turbulence is generated in the jet shear layer as long as the jet velocity remains high. Also, the gradual growth of the jet tip vortex (also known as the jet crown) has a considerable contribution to the turbulence generation. The rate of jet and ambient mixing can be directly related to the pre-chamber pressure as it influences the jet momentum and turbulence intensities.

Thus, more entrainment of cold gases to the hot jet is expected as the jet momentum rises. To further emphasize the effects of turbulent mixing, the ratio of turbulence energy dissipation to the turbulent kinetic energy, (ε/TKE), which varies inversely with the turbulence timescales. The maximum value of ε/TKE attained during the simulation time is provided in Fig. 4. The maximum ε/TKE ratio rises with jet momentum, increases mixing and shortens $\tau_{mix}$.

The competition between the two time scales can be inferred from Fig. 4. For the higher reactivity fuel, Fuel-HR, $\tau_{ch}$ is short enough to allow the mixing process to control the ignition progress. Therefore, as the jet momentum increases, ignition delay reduces due to the enhanced mixing and heat exchange between hot jet and cold ambient mixture. The overall trade-off between chemical and mixing time scale for the Fuel-HR shortens the ignition delay by increasing the jet momentum. In contrast, for the Fuel-LR, the chemical reactions are relatively slower and $\tau_{ch}$ seems to be controlling the ignition process. For higher values of jet momentum, the excessive mixing and jet quenching prevents ignition within the simulation time limit of 3 ms.

Another significant observation from Fig. 4 is the fluctuations of the HHR after the ignition onset at 4 and 6 bar pre-chamber pressures. The fluctuations are seemingly accompanied by the pressure wave-flame interactions, which can locally alter the burning rate via multiple effects. These effects are beyond the scope of this work.

Figure 5 is a plot of the time history of temperature distribution on the midplane crossing the nozzle and CVC chamber for the Fuel-LR and Fuel-HR, respectively. The OH iso-curves are overlaid on the temperature plots emphasizing the ignition moment. It appears that ignition is successful when OH mass fraction exceeds a threshold of about 0.007. The ignition kernel is generally located at the jet tip vortex where high entrainment of reactants into the hot jet is expected. Subsequently, the reaction region spreads towards the lateral surfaces of the jet. In these cases of a centered stationary jet, the ignition kernel occurs near the centerline, but it appears that the growth of the kernel and subsequent combustion propagation is highly influenced by the narrow confinement in

the CVC. Figure 5-top illustrates the ignition occurrence for the Fuel-LR under different jet momentum. As was addressed by the HRR in Fig. 4 for the Fuel-LR, successful ignition happens only for the 2 bar pre-chamber pressure around 2.2 ms while faster jets fail to ignite within the simulation time limit. It should be noted that the late ignition (later than 3 ms in the present study) may be considered unsuccessful in cyclic combustion devices with limited available time. When the ignition kernel fails to be formed at higher jet momentum, it is mainly due to the time scale argument made earlier. The Fuel-LR has a longer chemical time scale because of its lower hydrogen content. The hot jet at high jet momentum has a shorter mixing time scale. As discussed, higher jet momentum causes stronger turbulence and faster mixing with the cold environment. Thus, before the jet can ignite the Fuel-LR, it loses its thermal energy due to the excessive mixing rates.

As depicted in the Fig. 5-bottom for the Fuel-HR, evidence of ignition at 2 bar pre-chamber pressure appears around 2ms after the jet discharge. This delay is significantly reduced as the jet momentum increases, so that at 6bar, the ignition kernel is formed roughly at 0.8 ms. The higher concentration of hydrogen in the Fuel-HR seemingly allows the reactions to progress much faster than for the Fuel-LR. Consequently, once the appropriate temperature is attained by the fuel mixture due to mixing with hot jet, ignition takes place. It is also worthwhile to notice the development of perturbations on the flame front as the combustion proceeds. These effects develop in the form of twisting and distorting of the flame front which can generally extend the effective reaction area. The detailed calculations of the flame surface show that in some instances, the flame area can stretch 30 times larger than the channel cross section.

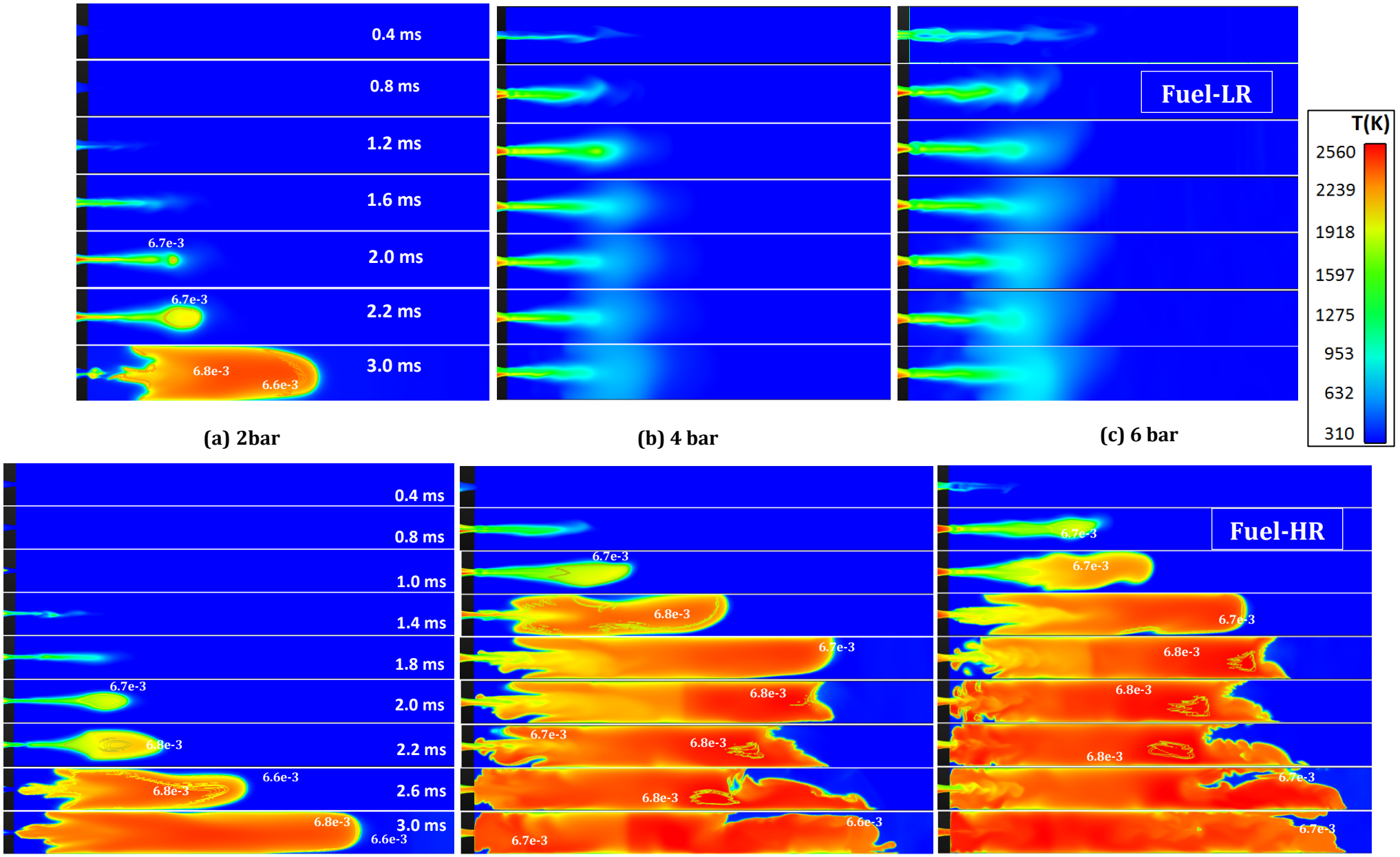


**Figure 5. History of temperature overlaid by OH iso-curves in CVC chamber for Fuel-LR (top) and Fuel-HR (bottom) at the pre-chamber pressures of (a) 2 bar, (b) 4 bar and (c) 6 bar.**
**Pictures are not to scale**

## 4. Ignition: A Function of Species Mass Fractions and Temperature

A goal of the study is to predict the time and possibly the location of ignition at operating conditions that are not simulated in detail as reactive flows. For instance, if the jet has a traversing motion or the CVC mixture is at elevated temperature, are we able to predict the ignitability of the mixture? Given the substantial cost of reactive flow simulations, is it possible to obtain sufficient guidance from non-reactive flow simulations of the mixing process?

Active radicals in the hot jet, such as $CH_x$ and OH, mix with the reactants and have been shown to play a significant role in the ignition process [18]. Thus, global reaction models for autoignition of unreacted mixture cannot quantify reaction rates. A simpler ignition criterion could be based on the presence of a certain concentration of reactants and temperature. By examining the simulation results with a post-processor, it is possible to track flow particles based on their origin whether it the pre-chamber or CVC. The authors studied the simulation results of successful ignitions in 12 cases [14] and discovered that at the ignition kernel (a sphere with critical size) the temperature, mass fraction originating in hot jet gases, and mass fraction originating in cold reactants in the CVC should be within certain ranges. Collecting all the data from previous simulations and aiming to develop a baseline, a Boolean ignition indicator called IGN was defined which represents the thermochemical properties of the ignition points achieved in the successful ignition cases. The variables and their limits were chosen as follows, based on a trial-and-error process of identifying the time and locations of ignition in the above-described simulations:

"IGN" = (0.1<Pre-chamber mass fraction<0.2) and (0.55<CVC chamber mass fraction<0.6) and

(Temperature>750 K)

When the ranges of all three variables are met simultaneously, cells are observed to have sustained reaction. It must be noted that the remainder of the mass in IGN criterion is constituted from the

diluent which is used to purge the nozzle assembly. In the configurations otherwise, the mass fractions need to be normalized.

IGN as an indicator could reduce the necessity of using computationally costly chemistry models, allowing non-reacting flow mixing study to establish likelihood of ignition. In support of the recommended temperature interval, the Semenov approach of thermal ignition suggests that for methane-hydrogen blend with activation energy about 180 kJ/mol and the mixture initial temperature of 750K, only 25K of temperature rise is sufficient for ignition occurrence [32]. Also, due to importance of active radicals on ignition at near-atmospheric initial condition of CVC, IGN is designed to represent the composition of the pre-chamber [33].

In order to examine the viability of the IGN criterion, an attempt is made to predict the ignition time for a case where the hot jet has a traversing motion, which has different jet physics. In a wave rotor combustor, for example, hot gas supplied by a pre-chamber or a prior-combusted chamber is transferred to a fresh-mixture chamber that is in motion relative to the transfer jet nozzle. Thus, depending on the rotational speed of the rotor, the CVC is experiencing a traversing jet along the end of the channel. Simulations of these cases were performed with and without inclusion of chemical reaction calculations, and ignition predictions from the two methods were compared. In the top plot of Figure 7 red markers represents IGN for the cells were the ignition criteria is met. It should be noted that the IGN is developed in the 'cold' flow simulation where the chemical reaction calculations are turned off. In the lower plots, the mid-plane temperature is shown for simulations with chemical reactions included, from which ignition can be directly predicted.

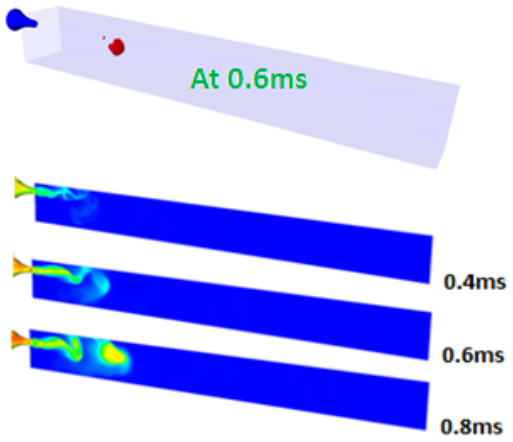


**Figure 6. Comparison of IGN prediction of the ignition time and location (top) with the corrosponding moment at the reacting flow simulation (bottom)**
**Jet traversing speed 12.8 m/s, Pre-chamber pressure 6bar, Fuel-HR**

As depicted in Fig. 6 (top), the full simulation predicts ignition at around 0.6 ms based on temperature field with chemical reaction included. Encouragingly, IGN predicts ignition at about the same time and location in the non-reacting flow simulations.

Table 4 is a comparison of the ignition time observed in combustion simulations along with the values predicted by IGN in the cold-flow simulations. The errors reported in Table 4 are inclusive of inherent uncertainties of IGN in predicting the actual ignition time as well as an additional 0.05 ms error contribution due to the time intervals at which the computational results are saved for postprocessing, due to storage limitations.

Another operating condition to be considered in applications of constant volume combustors is the CVC mixture temperature prior to jet injection. Combustion engines have varying levels of compression, and thus temperature of the mixture varies. In order to probe into the effect of elevated CVC temperature on combustion, a new set of simulations with and without chemical kinetic calculations were conducted in which the reliability of IGN in predicting the ignition time was examined. This comparison is also presented in Table 4, where Fuel-HR mixtures initially at

514 K are simulated. It is noted that the IGN variable substantially captures the strong downward trend in ignition delay time with increasing jet momentum.

**Table 4. Accuracy of IGN ignition predictor with introduction of jet traverse (top) and elevated CVC temperature (bottom)**

| Traversing Jet speed (m/s) † | Reacting flow Ignition time (ms) | IGN Ignition time (ms) | absolute error (ms) |
|---|---|---|---|
| 12.8 | 0.65 | 0.60 | 0.05 |
| 4.9 | 0.70 | 0.60 | 0.1 |
| 0.9 | 0.90 | 0.70 | 0.2 |

| | CVC initial temperature 514K‡ | Reacting flow Ignition time (ms) | IGN Ignition time (ms) | absolute error (ms) |
|---|---|---|---|---|
| Pre-chamber pressure (bar) | 2 | 1.70 | 1.75 | 0.05 |
| | 4 | 0.75 | 0.80 | 0.05 |
| | 6 | 0.70 | 0.60 | 0.2 |

†Pre-chamber pressure 6 bar, CVC temperature 300 K, Fuel-HR

‡ CVC elevated temperature 514 K, Fuel-HR

## Conclusion

The ignition and deflagration of air-$CH_4$-$H_2$ mixtures with initial standard pressure and temperature in a confined volume is numerically simulated and different operating conditions are studied with 3D simulations. The jet composition and temperature corresponded to the adiabatic equilibrium products of a slightly-rich fuel-air mixture. The following highlights were addressed in the present work:

- The pre-ignition development of the jet demonstrates self-preserving behavior as expected by the plug flow reactor model.

- The competition of the mixing and chemical time scales determines the success of ignition. Observations show the substantial decrease of the ignition delay with increasing the jet momentum for the hydrogen-dominated fuel blend, while its effect on the low-reactivity fuel blend is weakly in the opposite direction of quenching ignition.
- Experimental data for the same geometry and high-reactivity fuel blend as used in the simulations showed trend of ignition delay variation with jet momentum that was consistent with numerical model predictions, but with higher values that were expected due to suspected heat loss effects in the experiments that were not accounted in simulations.
- An ignition predictor variable (IGN) was developed and examined for estimation of ignition time and location while the cold flow was being simulated and no chemistry model is engaged. The IGN criterion is designed to benefit preliminary benchmarks for design of a CVC for combustion applications. IGN showed reliability for 3:7 and 1:1 methane-to-hydrogen ratios at near atmospheric pressures in comparison with chemical kinetic flow reactor calculations.
- The IGN criterion as established for non-traversing jet and for CVC mixture at room temperature was able to acceptably predict ignition delay for jets with traversing motion over a range of speeds, as well as for CVC mixtures with elevated initial temperature with a range of jet momentum, in comparison with chemical-kinetic flow reactor calculations.
- While the ignition is sensitive to the jet composition, IGN criterion presumes the jet composition to be the equilibrium products of a slightly rich-burn combustion at temperatures close to adiabatic flame.
- The IGN criteria used fixed values for three constituent variables across a significant variation in the physics-related variables of jet momentum, jet traverse speeds, and the chemistry-related variables of initial CVC mixture temperature and fuel reactivity.

- It is noted that the criteria might be only trusted for high aspect ratio and narrowly confined elongated combustors. Within the defined operating conditions, the IGN variable is shown to be able to predict the ignition time with precision ranging from 0.05-0.2 ms depending on the complexity of jet structure.

The study has been beneficial in suggesting a methodology for predicting ignition from lower-cost computations without chemistry calculations. The values of variables in the ignition criterion may be refined by further modeling and comparison with experiments, and by considering an expanded parameter space including varying the pre-chamber equivalence ratio, CVC chamber equivalence ratio, and nozzle diameter.

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## References

[1] Akbari, P., Nalim, R. and Mueller, N., 2006. A review of wave rotor technology and its applications. Journal of Engineering for Gas Turbines and Power, 128(4), pp.717-735.

[2] Oppenheim, A.K., 2004. Combustion in Piston Engines: Technology, Evolution, Diagnosis and Control. Springer.

[3] Gussak, L.A., Karpov, V.P. and Tikhonov, Y.V., 1979. The application of Lag-process in prechamber engines. SAE Technical Paper No. 790692.

[4] Wolanski, P., Gut, Z., Niedziela, W., Przastek, J. and Siwiec, S., 1997. Study of combustion dynamics in the research engine. SAE Technical Paper No. 972829

[5] Chinnathambi, P., 2014. Experimental Investigation on traversing hot jet ignition of lean hydrocarbon-air mixtures in a constant volume combustor. MS Thesis, Purdue University.

[6] Fink, Z.J. and Vanpee, M., 1975. Overall kinetics of hot gas ignition. Combustion Science and Technology, 11(5-6), pp.229-238.

[7] Carpio, J., Iglesias, I., Vera, M., Sánchez, A.L. and Liñán, A., 2013. Critical radius for hot-jet ignition of hydrogen–air mixtures. International Journal of Hydrogen Energy, 38(7), pp.3105-3109.

[8] Gentz, G., Thelen, B., Gholamisheeri, M., Litke, P., Brown, A., Hoke, J. and Toulson, E., 2015. A study of the influence of orifice diameter on a turbulent jet ignition system through combustion visualization and performance characterization in a rapid compression machine. Applied Thermal Engineering, 81, pp.399-411.

[9] Iglesias, I., Vera, M., Sánchez, A.L. and Liñan, A., 2012. Numerical analyses of deflagration initiation by a hot jet. Combustion Theory and Modelling, 16(6), pp.994-1010.

[10] Ghorbani, A., Steinhilber, G., Markus, D. and Maas, U., 2014. Numerical investigation of ignition in a transient turbulent jet by means of a PDF method. Combustion Science and Technology, 186(10-11), pp.1582-1596.

[11] Ghorbani, A., Steinhilber, G., Markus, D. and Maas, U., 2015. Ignition by transient hot turbulent jets: An investigation of ignition mechanisms by means of a PDF/REDIM method. Proceedings of the Combustion Institute, 35(2), pp.2191-2198.

[12] Sadanandan, R., Markus, D., Schießl, R., Maas, U., Olofsson, J., Seyfried, H., Richter, M. and Aldén, M., 2007. Detailed investigation of ignition by hot gas jets. Proceedings of the Combustion Institute, 31(1), pp.719-726.

[13] Brouillette, M., 2002. The Richtmyer-Meshkov instability. Annual Review of Fluid Mechanics, 34(1), pp.445-468.

[14] Khan, M.N., 2015. Three-dimensional transient numerical study of hot-jet ignition of methane-hydrogen blends in a constant-volume combustor. MS Thesis, Purdue University.

[15] Paik, K-Y., 2016. Experimental investigation of hot-jet ignition of methane-hydrogen mixtures in a constant-volume combustor. MS Thesis, Purdue University.

[16] Zhang, Y., Huang, Z., Wei, L., Zhang, J. and Law, C.K., 2012. Experimental and modeling study on ignition delays of lean mixtures of methane, hydrogen, oxygen, and argon at elevated pressures. Combustion and Flame, 159(3), pp.918-931.

[17] Goodwin, D.G., 2003. An open-source, extensible software suite for CVD process simulation. Chemical Vapor Deposition XVI and EUROCVD, 14(40), pp.2003-08.

[18] Karimi, A., Chinnathambi, P., Rajagopal, M. and Nalim, R., 2013. Hot-jet ignition of hydrocarbons and hydrogen in air: effect of jet chemical activity. Proceedings of the 49th AIAA/ASME/SAE/ASEE Joint Propulsion Conference.

[19] Nalim, M.R., Snyder, P.H. and Kowalkowski, M., 2016. Experimental Test, Model Validation, and Viability Assessment of a Wave-Rotor Constant-Volume Combustor. Journal of Propulsion and Power, Vol. 33, pp. 163-175.

[20] Richards, K.J., Senecal, P.K., Pomraning, E., 2013. CONVERGE Users Guide & Reference Manual (Version 2.2).

[21] Song, L. and Abraham, J., 2003. Entrainment characteristics of transient turbulent round, radial and wall-impinging jets: theoretical deductions. Journal of fluids engineering, 125(4), pp.605-612.

[22] Kazakov A, Frenklach M. Reduced reaction sets based on GRIMech 1.2. Available at http://www.me.berkeley.edu/drm/.

[23] Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, Jr., Vitali V. Lissianski, and Zhiwei Qin, http://www.me.berkeley.edu/gri_mech/

[24] Sung, C.J., Law, C.K. and Chen, J.Y., 2000. Further validation of an augmented reduced mechanism for methane oxidation: Comparison of global parameters and detailed structure. Combustion science and technology, 156(1), pp.201-220.

[25] Mansourian, M. and Kamali, R., 2017. Computational fluid dynamics analysis of a synthesis gas turbulent combustion in a round jet burner. Acta Astronautica, 134, pp.133-140.

[26] Steinhilber, G., Bykov, V. and Maas, U., 2017. REDIM reduced modeling of flame-wall-interactions: Quenching of a premixed methane/air flame at a cold inert wall. Proceedings of the Combustion Institute, 36(1), pp.655-661.

[27] Gholamisheeri, M., Wichman, I.S. and Toulson, E., 2017. A study of the turbulent jet flow field in a methane fueled turbulent jet ignition (TJI) system. Combustion and Flame, 183, pp.194-206.

[28] Turns, S.R., 1996. An introduction to combustion (Vol. 287). New York: McGraw-Hill.

[29] Issa, R.I., 1986. Solution of the implicitly discretised fluid flow equations by operator-splitting. Journal of computational physics, 62(1), pp.40-65.

[30] Diez, F.J., Sangras, R., Kwon, O.C. and Faeth, G.M., 2003. Erratum:"Self-preserving properties of unsteady round nonbuoyant turbulent starting jets and puffs in still fluids"[ASME J. Heat Transfer, 124, pp. 460–469 (2002)]. Journal of Heat Transfer, 125(1), pp.204-205.

[31] Mayinger, F., Jordan, M., Eder, A., Zaslonko, I.S., Karpov, V.P. and Frolov, S.M., 1999. Flame-jet ignition of fuel-air mixtures. Experimental findings and modeling. 17th International Colloquium on the Dynamics of Explosions and Reactive Systems (ICDERS), Heidelberg, Germany, July (pp. 25-30).

[32] Glassman, I., Yetter, R.A. and Glumac, N.G., 2014. Combustion. Academic press.

[33] Brower, M., Petersen, E.L., Metcalfe, W., Curran, H.J., Füri, M., Bourque, G., Aluri, N. and Güthe, F., 2013. Ignition delay time and laminar flame speed calculations for natural gas/hydrogen blends at elevated pressures. Journal of Engineering for Gas Turbines and Power, 135(2), p.021504.