

A Numerical Investigation of Ignition of Ultra-Lean Premixed H₂/Air Mixtures by Pre-Chamber Supersonic Hot Jet

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ABSTRACT

Gas engines often utilize a small-volume pre-chamber in which fuel is injected at near stoichiometric condition to produce a hot turbulent jet which then ignites the lean mixture in the main chamber. Hot jet ignition has several advantages over traditional spark ignition, e.g., more reliable ignition of extra-lean mixtures and more surface area for ignition resulting in faster burning and improved combustion burn time. Our previous experimental results show that supersonic jets could extend the lean flammability limit of fuel/air mixtures in the main chamber in comparison to subsonic jets. The present paper investigated the characteristics of supersonic hot jets generated by combustion of stoichiometric H₂/air in a pre-chamber to understand the ignition mechanism of ultra-lean mixtures by supersonic hot jets. Numerical simulations were carried out to examine the transient hot jets issued from six different nozzles (two straight nozzles, one converging nozzle, and three converging-diverging (C-D) nozzles) using a detailed H₂/air chemistry. The detailed flame propagation process inside the pre-chamber was investigated. Then the characteristics of the hot jets from six nozzles were compared, including the spatial and temporal distribution of velocity, vorticity, pressure, turbulence quantities, temperature, shock structures, and species concentrations. The results show that supersonic jets exhibit shock diamond structures. The static temperature rises after each shock and a significant temperature rise occur after the final shock. The location of this high-temperature zone is consistent with the experimental observations where ignition was initiated. The profile of Damköhler numbers based on the local flow properties was determined. A critical Damköhler number was found to be 11, below which the main chamber ignition would unlikely to occur. Additionally, the Damköhler number profiles help to explain why the two C-D nozzles with an area ratio of 4 and 9 could extend the flammability limit, whereas the C-D nozzle with an area ratio of 16 failed to do so.

KEYWORDS: Gas engines, Pre-chamber ignition, Supersonic jet ignition, Ultra-lean mixtures, Local Damköhler number, Extended flammability limit

CITATION: Biswas, S. and Qiao, L., "A Numerical Investigation of Ignition of Ultra-Lean Premixed H₂/Air Mixtures by Pre-chamber Supersonic Hot Jet," *SAE Int. J. Engines* 10(5):2017, doi:10.4271/2017-01-9284.

INTRODUCTION

Ever-stringent emission regulations have pushed engine manufacturers to pursue ultra-lean combustion technologies [1, 2]. However, when the fuel/air mixture is very lean, reliable ignition operation can be a challenge [3, 4]. One way to solve this problem is to use pre-chamber generated hot jet to ignite the lean mixture, rather than using a conventional spark plug [5, 6]. A small quantity of stoichiometric fuel/air is burned in a separate combustion chamber called the pre-chamber. The combustion products are then discharged into the main chamber filled with ultra-lean premixed fuel/air in the form of a hot turbulent jet. This technique is commonly used in large-bore natural gas engines. Compared to a conventional spark plug, the hot jet has a much larger surface area leading to multiple ignition sites which can enhance the probability of successful ignition and cause faster flame propagation and heat release.

Several studies [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29] have shown the potential of a turbulent hot jet to reliably ignite a lean mixture compared to a standard spark

ignition system. Gussak [7] is one of the earliest to propose the concept of using a hot jet made of incomplete combustion products containing chemically active species such as OH and HO₂. Chen and Ghoniem [8] studied the jet ignition characteristics using a hot flame jet of different shapes and speeds. Pitt et al. [9] showed that jet ignition resulted in shorter ignition delay and increased burn rates compared to a conventional spark system. Yamaguchi [10] investigated the effects of nozzle diameter on jet ignition. Wallesten and Chomiak [11] explored the possibility of extending the lean flammability limit by changing the spark position inside the pre-chamber. Most recently, Elhnawi and Teodorczyk [12] and Sadanandan et al. [13, 14] investigated ignition of H₂/air mixtures by a hot jet using Schlieren and OH LIF (Laser Induced Fluorescence) techniques. Toulson et al. [15, 16, 17, 18] examined combustion stability and flammability limit of different fuels (H₂, propane, and natural gas) in an optically accessible engine. Perera et al. [19] measured the ignition delay of ethylene/air ignited by a hot jet. Carpio et al. [20] and Karimi et al. [21] numerically studied the characteristics on the ignition behavior of lean H₂/air and CH₄/air

mixtures. Shah et al. [22, 23] investigated the effect of different pre-chamber volumes and orifice diameters on the performance of heavy-duty natural gas engines. Wang et al. [24] compared three different ignition methods - spark ignition, hot jet ignition, and pre-detonator - on a pulse detonation engine. All these studies show the great potential of hot jet ignition for extra-lean combustion. Nevertheless, most of the studies mentioned above used subsonic jets to ignite the lean mixture. In many cases, the velocity of the hot jet was not quantitatively measured or reported.

Only a few studies have been conducted to understand the effect of high-speed, transonic or supersonic hot reacting jets on ignition of ultra-lean fuel/air mixtures. Djebaili et al. [25] investigated ignition of lean H_2 /air mixture by a hot supersonic (Mach = 2.0) jet generated in a shock tube. They observed that the flame propagation velocity inside the main chamber increased significantly using supersonic jets. Boretti [26] numerically studied ignition of H_2 /air using a high speed (Mach = 0.7) compressible gas jet. The results showed that the ignition delay in the main chamber decreased with higher jet velocities. Chiera et al. [27] reached similar conclusions as Boretti [26] that higher velocity of the hot jet generated by pre-chamber combustion resulted in greater turbulence and multiple flame fronts, leading to faster combustion in the main chamber. However, there is a major potential concern with the usage of supersonic jets. Supersonic jets caused higher flow restriction between the pre-chamber and the main chamber could lead to longer 'residence time' of pre-chamber combustion products with a risk of deactivation before they are ejected into the main chamber.

However, the potential advantages of the supersonic hot jet from these previous limited studies motivated the authors to explore the concept of using supersonic hot jets to ignite ultra-lean mixtures. The authors developed an experiment [28, 29] which used a dual-chamber design to compare the ignition characteristics of subsonic jets versus supersonic jets. They found that the supersonic jets not only shortened the ignition delay but also extended the lean flammability limit of H_2 /air mixture in the main chamber, as compared to the subsonic jets. For example, the lean limit achieved by subsonic jets using straight nozzles was found to be $\phi = 0.31$. Supersonic converging-diverging nozzles, however, can extend this limit to $\phi = 0.22$. Moreover, radiation intensity measurements of the hot jets showed the presence of a high-temperature zone at the downstream of the shock structures for the supersonic jets. Ignition in the main chamber was initiated near to that high-temperature zone. Our previous study [28] on the fundamental mechanism of hot jet ignition showed that both temperature and velocity of the hot jet govern the ignition process in the main chamber. Whether ignition can happen or not depends on the competition between turbulent mixing and ignition chemistry. For ignition using supersonic jets, there are additional complexities due to the presence of shock structures and the interactions between the shocks and the cold surroundings. It is essential to understand the physics behind the supersonic jet ignition process - how and why supersonic jets can extend the lean flammability limit of the main chamber mixture.

Note that we have limited our pre-chamber condition to stoichiometric throughout the current study. The ignition mechanism of the main-chamber mixture may be different for fuel-rich pre-chamber conditions.

Gussak [7] proposed using a rich mixture ($\phi = 1.42 - 2.5$) in the pre-chamber to produce a low temperature torch of incomplete combustion products containing chemically active species such as CH_3 , H , C_2 , aldehyde and peroxide. It was found the main chamber flammability limit widens with fuel rich pre-chambers. Along with fuel rich pre-chamber, Gussak also explored the effect of pressure difference across the two chambers dP and the nozzle diameter on the resulting vortex formation in the main chamber. It was found that the mixing vortices became smaller with an increase in dP , and below a critical nozzle size, the vortices are unable to serve as sites for mixing and ignition in the main chamber. Nevertheless, we must note that the nozzle diameter in Gussak's study was around 10 mm, which was much larger than those in the present study, 1.5 - 3 mm.

Motivated by the above, numerical simulations were carried out using the commercial CFD code, ANSYS Fluent 15.0 to simulate the flame propagation process within the pre-chamber and the penetration process of the transient turbulent hot jet issued from the pre-chamber into the main chamber. The goal was to understand why supersonic jets can extend lean flammability to achieve leaner combustion in the main chamber, which potentially can further reduce NOx emissions in gas engines. Here we chose hydrogen as the fuel due to its simple chemistry and potential as an alternative fuel. The simulations followed the exact same conditions of the experiment [29], in which six different nozzles including two straight nozzles, one converging nozzle, and three converging-diverging (C-D) nozzles were tested, and their performance was compared. For each nozzle, we examined the characteristics of the hot jet, including the spatial and temporal distributions of velocity, vorticity, Mach number, pressure, temperature, and shock structures. Additionally, the local Damköhler numbers of the reacting fuel/air mixture as a function of time and location were calculated for different types of nozzles just before ignition took place in the main chamber. This comparison of local Damköhler numbers helped to reveal the fundamental mechanism of supersonic jets extending the lean flammability limit.

NUMERICAL METHOD

Experimental Conditions and Major Findings

The primary objective of this study is to understand the effect of nozzle geometry on the ultra-lean ignition limit of H_2 /air. This knowledge is crucial to explain how supersonic nozzles can extend the lean flammability limit compared to straight nozzles. The initial and geometric conditions used for the numerical simulations are identical to those in our previous experiment [29]. The experimental setup was described in detail in [29], and thus only a brief description is presented here. A small volume stainless steel pre-chamber was mounted on the top of a carbon steel main chamber. The main chamber to pre-chamber volume ratio is 100:1. A stainless steel orifice plate with various nozzle designs was placed between the two chambers to separate them. Six different nozzles as illustrated in Figure 1 were tested. The geometric parameters, as well as the measured main-chamber lean flammability limit, ϕ_{limit} for each nozzle, are summarized in Table 1. Note that the straight nozzle, Nozzle 2, had a larger diameter, 3 mm, whereas all other nozzles had a throat diameter of 1.5 mm. Since the mass flow rate is the same, the effective flow area i.e. throat area of Nozzle 2 would have a higher

mass flux flowing through the pre-chamber to the main chamber. Mixtures in both the chambers were initially kept at room temperature. The stoichiometric H_2 /air mixture in the pre-chamber was ignited by an electric spark generated at the top of the pre-chamber. Once the spark ignited the pre-chamber mixture, the combustion products started to enter into the main chamber in the form of a hot jet which then ignited the ultra-lean main chamber.

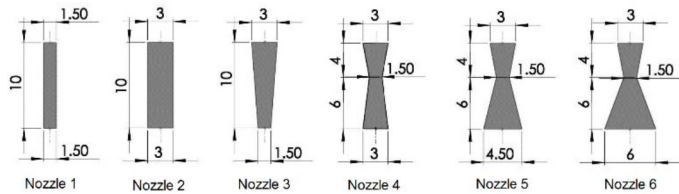


Figure 1. Schematic of different types of nozzle designs. All dimensions are in millimeter [29].

The lean limit for each nozzle was found by gradually reducing the H_2 /air equivalence ratio inside the main chamber until ignition could not occur anymore. Note the H_2 /air equivalence ratio of the pre-chamber mixture was fixed at $\phi = 1$ for all cases, whereas the H_2 /air equivalence ratio of the main chamber mixture was varied. Table 1 shows the lean limit ϕ_{limit} of the main chamber mixture for the six nozzles. As can be seen, ϕ_{limit} was extended for the supersonic nozzles compared to its straight counterpart. Out of the four supersonic nozzles we tested, nozzle 4 and 5 with an area ratio of 4 and 9 respectively resulted in the lowest flammability limit, $\phi_{limit} = 0.22$ and 0.23. We observed in supersonic jets the static temperature increased after each shock and a significant temperature rise occurred after the final shock. It was observed that the main chamber ignition started from this high-temperature region. While the C-D nozzles with an area ratio of 4 and 9 extended the flammability limit, the C-D nozzle with an area ratio 16 failed to do so.

Table 1. Nozzle type, dimension, and the measured lean limit ϕ_{limit} for the six nozzles used in the hot jet ignition experiment and the numerical simulations.

Nozzle #	Type	d_{inlet} mm	d_{throat} mm	d_{exit} mm	$\frac{A_e}{A_t}$	ϕ_{limit}^*
1	Straight	1.5	1.5	1.5	—	0.34
2	Straight	3	3	3	—	0.31
3	Convergent	3	—	1.5	—	0.29
4	C-D	3	1.5	3	4	0.22
5	C-D	3	1.5	4.5	9	0.23
6	C-D	3	1.5	6	16	0.29

Simulation Domain and Boundary Conditions

We aimed at computing the flame propagation process inside the pre-chamber and the penetration process of the transient hot jet until ignition occurs in the main chamber. In other words, the simulation would stop when ignition and flame propagation start in the main chamber. Figure 2 (a) shows the 2D computational domain and different types of boundary conditions. Due to symmetry, only half of the domain was modeled. The computational domain was divided into three zones, namely the pre-chamber zone, the nozzle zone and the main chamber zone, respectively. The pre-chamber has dimensions of L (length) x D (diameter) = 88.9 mm x 19.05 mm. The dimensions of the nozzle connecting the two chambers are already

reported in Table 1. The main chamber has dimensions of L (length) x D (diameter) = 304.8 mm x 101.6 mm. The entire domain was discretized using quadrilateral cells. Figure 2 (b) shows the mesh of the entire computational domain. Figure 2 (c) presents a magnified view of the meshed connecting nozzle between the pre-chamber and the main chamber. The minimum grid size in the initial mesh was 0.05 mm. However, to capture a shock, the solution-adaptive dynamic mesh refinement feature was used to resolve shock structures. The mesh was refined based on the pressure gradient present in the flow. Dynamic mesh adaptation was applied at every 20 iterations out of 100 per time step. Mesh or grid independence study was conducted by running the model on two different refined meshes - coarser and finer than the original mesh. The coarser and finer mesh consisted of approximately 350,000 and 700,000 cells respectively. The pressure rise in the main chamber (point P₁ and P₂ in Figure 2 (a)) was monitored for these two mesh sizes. The spatial velocity profiles inside the nozzle were also compared for these two different mesh sizes. It was found that the solutions were nearly identical for these two different mesh sizes.

An axisymmetric boundary condition was used at the centerline, while everywhere else wall boundary conditions were applied. The initial wall temperature was constant at 300 K with non-slip boundary condition. Initially, the pre-chamber mixture was set at the stoichiometric condition, and the main chamber mixture was at the ultra-lean condition. At $t = 0$ the premixed H_2 /air mixtures at both chambers were set to be at 300 K. The material of the pre-chamber and nozzle walls is stainless steel (SS316) and the main chamber wall material is carbon steel (C-1144) identical to the experimental conditions. An adiabatic wall of the pre-chamber was considered for the simulations. We performed simulations that included heat transfer through the walls. But, we found the effect of heat transfer through pre-chamber wall is insignificant.

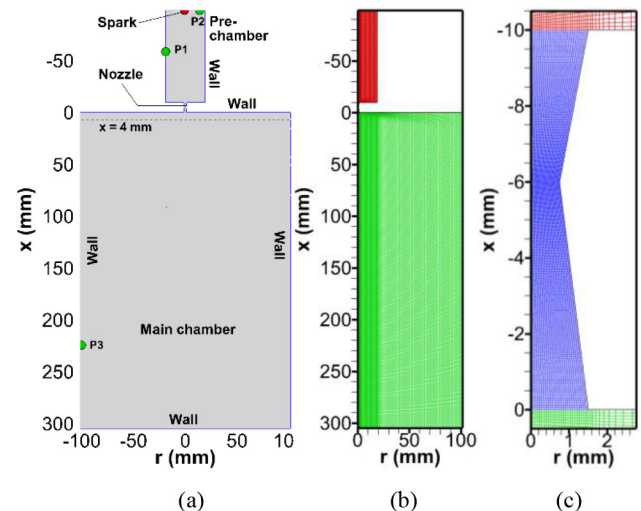


Figure 2. (a) Schematic of the computational domain; (b) the computational domain and three different zones, namely pre-chamber, nozzle and main chamber zones; and (c) the magnified view of the mesh of the connecting nozzle.

Both chambers were quiescent at the beginning of the simulation. At the beginning of the simulation, a spark with an energy of 100 mJ was supplied at the location (2, 0) mm within the pre-chamber to initiate ignition. At first, a laminar flame was observed

to propagate outwardly. As the pressure in the pre-chamber was building up, part of the unburned gasses in the pre-chamber was pushed out into the main chamber. To separate the two chambers with different equivalence ratios, a lightweight, 25 ± 1.25 -micron thick aluminum diaphragm was used in the experiment. When the pressure difference between the two chambers reached a threshold, the diaphragm ruptured resulting in a transient hot jet penetrating into the main chamber. A series of tests were conducted, and the pressure difference between the two chambers was found to be 0.21 MPa, above which the diaphragm bursts open. To match the experimental conditions, a user-defined step function was provided at the nozzle inlet in the simulations. Below the threshold pressure difference, 0.21 MPa, the inlet was closed, and it started operating above the threshold pressure difference. At around 2.15 ms, the pre-chamber pressure difference between two chambers reached 0.21 MPa, and the hot combusted products from the pre-chamber combustion were pushed out into the main chamber in the form of a turbulent hot jet. The simulations stopped at the instance just before ignition started in the main chamber. This time, when the simulation would stop, was measured experimentally and fed into the numerical model. The simulations did not include the ignition and combustion processes in the main chamber, and the focus was on the characteristics of the turbulent hot jet.

Governing Equations

The governing equations that describe transient chemically reacting compressible flows are the Unsteady Reynolds Time-Averaged Navier-Stokes (U-RANS) equations coupled with mass, energy, and species conservation equations [30, 31]. There are $(N - 1)$ species conservation equations, where N is the total number of species. These partial differential equations can be written as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \quad (1)$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + \delta_{ij} P - \sigma_{ij}) - \rho g_j = 0 \quad (2)$$

$$\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} (\rho H u_j + q_j - \sigma_{ij} u_i) = 0 \quad (3)$$

$$\frac{\partial}{\partial t} (\rho Y_m) + \frac{\partial}{\partial x_j} (\rho Y_m u_j + \rho Y_m V_j) = \dot{w}_m \quad (4)$$

where t is time, ρ is the density, P is the pressure, u is the velocity, E is the total energy, H is the total enthalpy, σ_{ij} is the stress tensor, q_j is the heat flux vector, δ_{ij} is the Kronecker delta, and Y_m , V_j and $\dot{w}_m$ are the mass fraction, diffusion velocity, and the production rate of the m^{th} species, respectively. The time-averaged conservation equations are obtained by decomposing each flow variable, ρ , u_i , P , σ_{ij} , E , H , q_i , Y_m , $\dot{w}_m$ into a mean and fluctuating part and then plugging into Equations 1, 2, 3, 4. A mass weighted average, known as the Favre average, is used to decompose the dependent variable f into a mean $\bar{f}$ and a fluctuating f'' part.

$$f = \bar{f} + f'' \quad (5)$$

$$\bar{f} = \frac{1}{\bar{\rho}} \lim_{\Delta t \rightarrow \infty} \frac{1}{\Delta t} \int_{t_0}^{t_0 + \Delta t} \rho f dt \quad (6)$$

Substituting the decomposed variables into Equations 1, 2, 3, 4 and using Favre averaging as shown in Equation 6 yield the desired time-averaged equations:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial t} (\bar{\rho} \bar{u}_j) = 0 \quad (7)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i) + \frac{\partial}{\partial t} (\bar{\rho} \bar{u}_i \bar{u}_j + \delta_{ij} \bar{P}) = \frac{\partial}{\partial x_j} (\bar{\sigma}_{ij} - \bar{\rho} \overline{u_i'' u_j''}) \quad (8)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{E}) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{H} \bar{u}_j) = \frac{\partial}{\partial x_j} (\bar{\sigma}_{ij} \bar{u}_i + \bar{\sigma}_{ij} \bar{u}_i'' - \bar{q}_j - \bar{\rho} \overline{H'' u_j''}) \quad (9)$$

$$\frac{\partial}{\partial t} (\bar{\rho} \bar{Y}_m) + \frac{\partial}{\partial x_j} (\bar{\rho} \bar{Y}_m \bar{u}_j) = \bar{w}_m - \frac{\partial}{\partial x_j} (\bar{\rho} \bar{Y}_m \bar{V}_j + \bar{\rho} \overline{Y_m'' u_j''}) \quad (10)$$

All the terms on the right-hand side of Equations 7, 8, 9, 10 require modeling assumptions. The time averaged molecular stress tensor, $\bar{\sigma}_{ij}$ as shown in Equations 8 and 9 can be modeled by ignoring the effects of turbulent fluctuations on the molecular viscosity, μ as

$$\bar{\sigma}_{ij} = \mu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \mu \frac{\partial \bar{u}_k}{\partial x_k} \quad (11)$$

The second term in right-hand side of the decomposed energy equation, $\bar{\sigma}_{ij} \bar{u}_i''$ can be correlated with the mean turbulent kinetic energy, $\bar{k} = \bar{u}_i'' \bar{u}_i'' / 2$ using following approximation

$$\frac{\partial}{\partial x_j} (\bar{\sigma}_{ij} \bar{u}_i'') = \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \bar{k}}{\partial x_j} \right) \quad (12)$$

The time-averaged heat flux vector, $\bar{q}_j$ usually, contains contributions from heat conduction and an energy flux term due to inter-species diffusion. $\bar{q}_j$ can be written as

$$\bar{q}_j = -\lambda \frac{\partial \bar{T}}{\partial x_j} + \sum_{m=1}^N \bar{\rho} Y_m V_j h_m(T) \quad (13)$$

The total energy, E is the sum of the internal energy, $e = c_v T$ and the kinetic energy, $k = u_i u_i / 2$. The total enthalpy is the sum of total energy, E , and P/ρ . Pressure, P is given by the ideal gas equation, $P = \rho RT$, where $R = R_u \sum_{m=1}^N Y_m / W_m$ is the gas constant, W_m is the molecular weight of the m^{th} species, and R_u is the universal gas constant. Thus, the total enthalpy, H can be expressed as, $H = h + u_i u_i / 2 + P/\rho$. The diffusion velocity of the m^{th} species is usually evaluated from Fick's law of diffusion and can be expressed in the following form

$$V_j = -\frac{D_m}{Y_m} \frac{\partial Y_m}{\partial x_j} \quad (14)$$

Here, D_m is the mass diffusivity of the m^{th} species relative to the mixture.

These governing equations, Unsteady Reynolds Averaged Navier-Stokes (U-RANS) equations, were solved in the 2D axisymmetric domain as shown in Figure 2 using the commercial code ANSYS Fluent R15.0. Each simulation was run in parallel on 4 nodes; each node contained 16 processors; a total of 64 processors were used per simulation. The computational time for each simulation is about 6 - 7 days to obtain a simulation time of approximately 50 milliseconds. Details of the turbulence modeling, turbulence-chemistry interaction, and numerical solver setting are discussed in the subsequent sections.

Turbulence Modeling

The Reynold's Stress Models (RSM) [32], a higher-level turbulence model was used to calculate individual Reynolds stresses, $\bar{\rho} u_i'' u_j''$. RSM has the superior competency to predict complex flows accurately as it accounts for the effects of swirl, rotation, and streamline curvature in a more rigorous manner than other turbulence models like $k - \epsilon$ [33, 34] or $k - \omega$ [35]. For instance, in flows with high degrees of anisotropy, significant streamline curvature, flow separation, zones of recirculating flow or flows influenced by rotational effects, the performance of eddy viscosity models are less satisfactory. In such flows, Reynolds stress equation models offer better accuracy [36, 37, 38, 39, 40]. However, RSM generally suffers from numerical stability issues due to the complexity of the modeled terms. However, the accuracy of RSM models is limited by the closure assumptions employed to model various terms such as the turbulent diffusive transport and pressure-strain terms in the Reynolds stress transport equation. A gradient-diffusion model of Daly and Harlow [41] was used to model turbulent diffusive transport. A pressure-strain model proposed by Speziale, Sarkar and Gatski [42] was chosen due to its superior performance for axisymmetric expansion and contraction.

Chemistry Modeling

A detailed chemistry model including 9 species and 21 reactions [43] was used for H_2 /air in the present simulations. Thus, we had 9 species equations to solve along with mass, momentum, and energy equations. To calculate mole fractions of these 9 species equations, the production rate of the species was needed. The species production rate was determined by the forward and backward reaction rates computed in ANSYS Fluent from the provided detailed chemical mechanism. The detailed chemical mechanism supplied the pre-exponential factor, temperature exponent, the activation energy for the reaction using Eddy-dissipation-concept (EDC) model necessary to calculate reaction rates. The turbulence-chemistry interaction was modeled using the Eddy Dissipation Concept (EDC) [44] model. The EDC model assumes that reaction occurs in small turbulent structures, called the fine scales. This model has the capability to include detailed chemical reaction mechanisms accurately.

A burning velocity model is necessary to calculate the burning velocities of H_2 /air at different locations and time steps in the simulation. For both adiabatic and non-adiabatic combustion models, the properties of the unburned fuel/air mixture, such as thermal conductivity, mass diffusivity, viscosity, and laminar flame speed, needed to be assigned. We needed to know the spatial variation of laminar burning speed to calculate local Damköhler numbers. To consider the effect of pressure and temperature variation within the domain this empirical model of laminar flame speed was used. The laminar burning velocity of H_2 /air mixture depends on the equivalence ratio, pressure, and temperature. Based on the burning model proposed by Iijima and Takeno [45], the laminar burning velocity, $s_L(T, P)$ of H_2 /air can be expressed as

$$\frac{s_L(T, P)}{s_L^0(T_0, P_0)} = \left(\frac{T}{T_0}\right)^{\alpha_1} \left[1 + \alpha_2 \ln\left(\frac{P}{P_0}\right)\right] \quad (15)$$

where $s_L^0(T, P)$ denotes the laminar burning velocity at the reference condition T_0 and P_0 , $\alpha_1 = 1.54 + 0.026(\phi - 1)$ and $\alpha_2 = 0.43 + 0.003(\phi - 1)$. Both α_1 and α_2 have a weak dependence on the equivalence ratio, ϕ . This empirical Equation 15 for the burning velocity of H_2 /air was obtained by fitting to the experimental data of H_2 /air mixtures in the equivalence ratio range of $\phi = 0.5 - 4$, temperature range of 291 K to 500 K, and pressure range of 0.5 to 25 atm.

Numerical Details

The compressible Navier-Stokes equations were solved using a pressure-based solver in which the pressure and velocity were coupled using the SIMPLE [46] algorithm. At the beginning of the simulation for a few milliseconds, a first-order upwind discretization scheme was used for the convective terms and turbulent quantities to obtain a stable, first order accurate solution. Once a stable solution was reached, we switched the discretization scheme to third order MUSCL [47] for an accurate solution. However, this higher order discretization scheme increased computation time significantly. The least squares cell-based gradient calculation scheme, which is known for accuracy and yet computationally less expensive, was chosen over the node-based gradient for the spatial discretization. A second order discretization scheme was used for pressure. The solution-adaptive mesh refinement feature was used to resolve shock structures. A dynamic adaptation of the pressure gradient was implemented to refine the mesh near the shock or to coarsen it wherever needed. A fixed time step of $t = 10^{-5}$ second was used to resolve the chemical timescale, which was estimated to satisfy the Courant-Friedrichs-Lewy (CFL) condition for numerical stability. To attain a stable solution, we used a Courant number around unity. The second order implicit scheme was used for time integration of each conservation equation.

RESULTS AND DISCUSSION

Numerical results from six different nozzle geometries are presented here. Quantitative comparison among different geometry nozzles was performed to explain the superior performance of supersonic jets over subsonic jets. At first, the flame propagation process within the pre-chamber is discussed in detail. Then the spatial variation of velocity, vorticity, shock, Mach number, species concentration, and

temperature are presented and discussed in depth. Lastly, the local Damköhler numbers are calculated based on the local flow properties just before ignition in the main chamber, which helps to understand the physics of ignition process by supersonic hot jets.

Validation

In the experiment [29], the pressure histories of both chambers were recorded using high-speed pressure transducers. Additionally, the temperature of the jet at several locations downstream of the nozzle exit was measured using the Hot Wire Pyrometry (HWP) technique. HWP provides a time-resolved temperature field along a line during jet propagation by measuring the blackbody radiation intensity through a bandpass filter of $3.92 \pm 0.03 \mu\text{m}$ using an infrared camera (FLIR SC6100) with an InSb detector. These measurements were averaged over a very brief time, 50 microseconds, which is the infrared camera integration time. Here we have compared the computed and measured pressure histories of the two chambers as well as the temperature profiles of the jet with the intent to provide a validation of the computational method.

As depicted in Figure 2 (a), in the numerical simulations, the pressure history of the pre-chamber was monitored at two locations P_1 and P_2 , while the main chamber pressure history was monitored at location P_3 . These locations were chosen because they were the same locations where the pressure transducers were installed in the experiment. Figure 3 compares the measured and computed pressure histories in the pre-chamber, which agree well. Both show that after a short ignition delay, the pre-chamber combustion initiated and the pressure started rising. The peak pressure, which is almost 6 times the initial pressure, occurred at

about 9 milliseconds after ignition. Afterward, pressure started to drop because the combustion products had been pushed into the main chamber. The computed pressure around the peak is slightly higher than the experimentally measured values, which may be because heat loss (from the pre-chamber to the surroundings) was neglected in the simulations. We performed simulations that included heat transfer through the walls and found the effect of heat transfer through the pre-chamber wall is insignificant. Upon close examination of the radial temperature profiles at two separate locations inside the pre-chamber just prior to the ignition in the main chamber, we noticed even though there is a slight difference in near wall temperature distribution, the centerline temperature of the pre-chamber remains same. Thus, we did not include heat transfer through pre-chamber walls for the rest of the simulations.

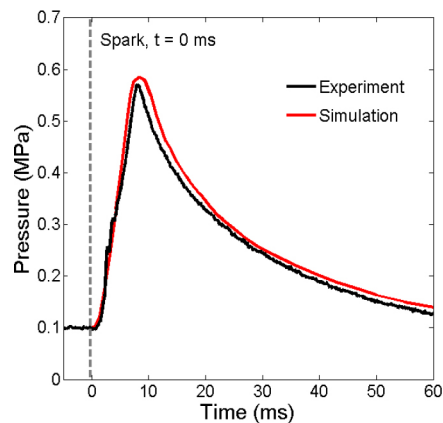


Figure 3. Comparison of the measured and computed pre-chamber pressure histories.

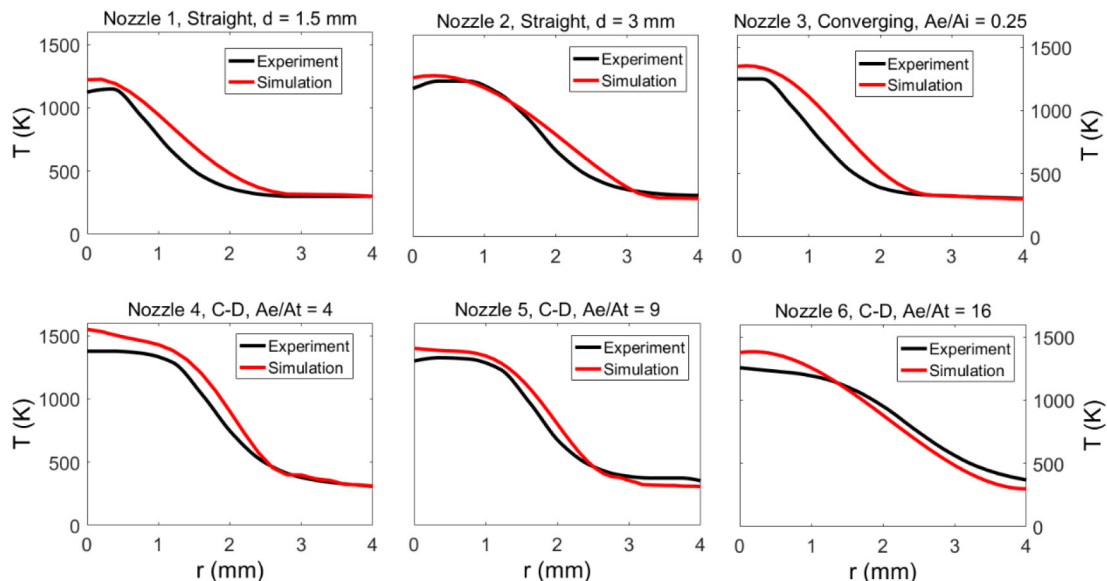


Figure 4. Comparison of computed and measured temperature profiles of the hot jet at $x = 4 \text{ mm}$ downstream of the nozzle exit just prior to the main chamber ignition for respective nozzles.