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Numerical study of hydrogen jet in methane / air premixed atmosphere

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Abstract: The work presented a numerical study on the transient characteristics of under-expanded hydrogen jets from a cylindrical nozzle. The finite-volume solution was adopted in the two-dimensional simulation of high-pressure chocked hydrogen jets, by solving the Navier-Stokes equations for gas phase flow. Numerical analyses were respectively performed over the micro level to characterize the fine structures, and over macro levels to explore the key global parameters of the gaseous jets. Parameterization work was conducted in terms of the microscopic characteristics of jets, such as, the length of jet core, the diameter of jet vortex, and the key global parameters, i.e. the penetration and the steady fuel injection rate. The effects of the injection parameters on the micro-structure and macro characteristics were hence quantified.

Keywords: Under-expanded hydrogen jets; Core length; Penetration; Mass injection rate; Nozzle pressure ratio.

1. Introduction

With the wide application of gaseous fuels direct injection in engines, the study on high-pressure gas jets has attracted intensive attention [1-3]. Compared to liquid fuels, the lighter gaseous fuels remain lower viscosities and higher diffusion coefficients, resulting in that the behaviors of their high-pressure jets are obviously different from that of liquid sprays[4]. The nozzle pressure ratio, NPR, commonly defined as the ratio of the upstream reservoir (nozzle) pressure to the ambient pressure, was found to be one of the most important factors to the characteristics of gas jets. With the change of NPR, gas jets could be presented as subsonic, moderately under-expanded and highly under-expanded flows respectively[5]. 1.95 is an critical value for most diatomic gases [6]. When NPR>1.95, gas jets would become under-expanded due to the chocked phenomenon at the nozzle exit, and many complicated flow behaviors, such as shock waves and Mach disks could be observed [7, 8]. It was reported that, there are great similarities in the flow structure of under-expanded jets [9, 10]. The flow field of an under-expanded gas jet was segmental and can be divided into three parts, i.e. the initial, the transient and the fully developed regions[11], according to the jet velocity or jet concentration. The initial region is normally defined as an inviscid near-nozzle core region with a uniform mean velocity, while the close-neighbor domain with gradually decreased velocities can be viewed as the transient zone. For both the initial and transient regions, the flow is at the near-field of nozzle and its structures are primarily governed by the shock. However, the fully developed region is at the far-field of the gas flow, which is often approximated by an equivalent flow behaving like a point-source vortex ball[9]. There are obvious characteristics differences between the near-field and the far-field of a gaseous jet flow, therefore, the flow field of high-pressure gas jets could also be differentiated as that in near-field and far-field [12].

Hydrogen (H2) is a lighter, more diffuse gas fuel than natural gas. Its direct injection has been viewed as an optimal technological path for practice utilization in engines [13, 14]. Therefore, the studies on high-pressure hydrogen jets has also attracted somewhat attention. Yip et al.[15] and Péneau et al. 16] explored the shock and Mach structures in under-expanded hydrogen jets. Mansor et al. [17] compared the penetration behaviors of hydrogen jets in argon and nitrogen atmospheres. Deng et al.[18]measured the penetrations of steady high-pressure hydrogen and oxygen jets in argon atmosphere. They found that, hydrogen jets show relatively greater jet penetration lengths and dispersion angles, compared to oxygen jets, while oxygen jets present about 2.43-2.98 times of entrainment rate to that of hydrogen jets, because of the lower volume flow rate of oxygen jets.

Generally, natural gas (NG) or methane is the most commonly used gaseous fuel, a number of fundamental studies were thus conducted for them. However, the attention paid upon the study of high-pressure hydrogen jet is not compatible with the potential application of hydrogen. The characteristics including the micro and macroscopic characteristics of high-pressure hydrogen jets under engine-related conditions were not well-known. The present work aims to find some transient flow-fields and flow properties of the under-expanded hydrogen jets under different NPR conditions, for stopping the urgent theoretical gaps in the direct injection engine application of hydrogen. The numerical study is conducted by solving the governing equations of high-pressure gaseous jets. The transient properties of hydrogen jets is analyzed in terms of the mass injection rate, the lengths of penetration and core, and vortex scale.

2. Modeling and analysis methodology

In this numerical work, the Navier-Stokes equations for gas phase flow, consisting of the conversation equations of mass, momentum and energy, and the specie transport, were solved using the finite-volume solution by ANSYS CFX Code. In order to achieve rapidly convergent jet solution, all species and gas were viewed as ideal gas. Mass diffusion predicted using the kinematic theory, and the computation of the density, thermal conductivity and viscosity of the mixture follows the law of gas mixing. The high-pressure hydrogen is delivered to the gas injector and then jets into a constant volume vessel

(CVV). The surrounding gas in the CVV is air. For simplify the computation, the dynamic effects of the internal flow in the injector was not considered, and the computational domain only consists of the CVV system and the internal flow field of the nozzle, as marked by dark meshes in Fig.1.

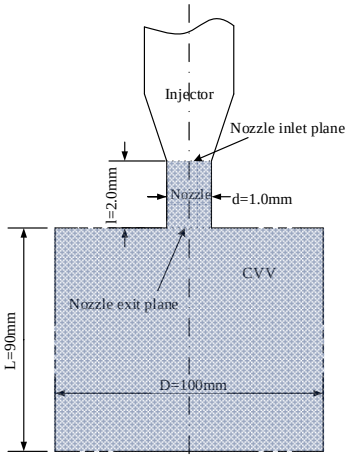


Fig 1. Schematic setups of the injector and the constant volume vessel.

The surrounding air in the CVV are set to be quiescent. The RNG K-ε turbulence model was adopted into the computation, to simulate the turbulence induced by the high-pressure ejected jets. The standard wall function were adopted for considering the shear effect of the gas flow in the nozzle. The second-order upwind scheme was selected for spatial discretization, and then density-based transient solutions were implemented to yield jet structure, where the time step is set to be 1.0 us. The previous studies[19,20] and the predicted results suggested that this time step is fine enough to capture the development of the dynamic structure of high-pressure gaseous jets. The effects of jet temperature was not studied. The temperatures of hydrogen jets and the ambient gas were both fixed at 300K. The present work is primarily performed to explore the effects of the injection pressure and the ambient pressure on jet characteristics. Therefore, the injection pressures varied from 3.0 to 6.0 MPa, and three ambient pressure in the CVV, i.e. 0.5, 1.0 and 1.5MPa were introduced into the jet computation. NPR ranges from 2.0 to 12.0. All are greater than 2.0, that is to say, all predicted jets would be initially chocked and under-expanded.

The simulation work was implemented under two dimensions condition. It was reported that the mesh quality has significant influence on the convergence and even the accuracy of jets modeling[21]. Considering that the computation domain is not too large, the fixed grid 0.2mm was adopted. The computational results showed the mesh scale is enough fine to achieve a good trade-off between computational accuracy and convergence rate.

3. Results and discussion

Fig.2 shows the change curve of three different η0 values of the jet pressure (Pj) 6MPa of the high-pressure hydrogen jet at the back pressure 0.5, 1, 1.5MPa in the methane / air premixed atmosphere over time, where η0 is the value of NPR.

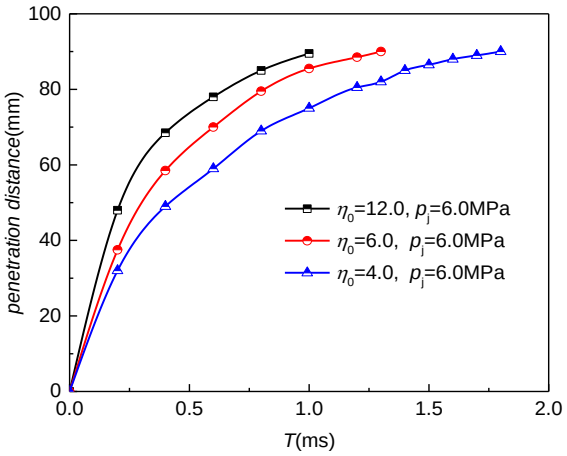


Fig 2. Hydrogen jet with different environmental backpressure runs through the distance

It can be seen from the figure that in the initial stage of jet development, the penetration distance of jet increases rapidly with time. With the growth of jet time, although the penetration distance of jet gradually increases with time, its growth rate is obviously smaller than the initial stage of jet development.With the gradual increase of the back pressure in the internal environment, the resistance of the ambient gas increases, the gas fuel jet decreases, the initial velocity decreases, the penetration distance of the jet decreases.

Fig.3 shows the variation of jet core length with the elapsed injection time. For all modeled jets, the curves of core length illustrate a rapid increase within about 0.20 ms, and then stay at a steady value. The steady core length is defined as LC,However, the jet with the higher NPR shows a relative greater Lc and the jets with a same NPR illustrate comparable Lc curves, indicating that LC is an NPR–related eigenvalue for high-pressure gaseous jets.

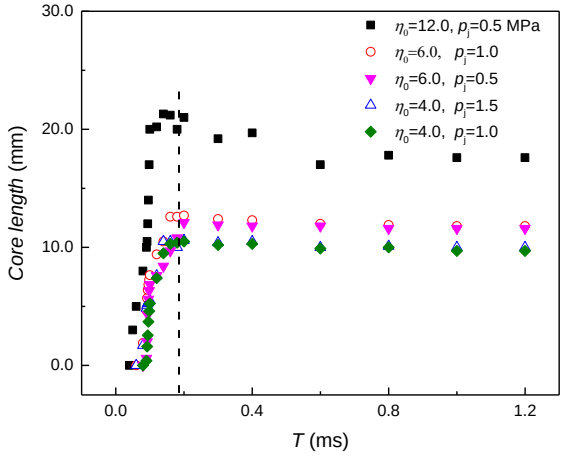


Fig 3. Variation of jet core length with the elapsed time

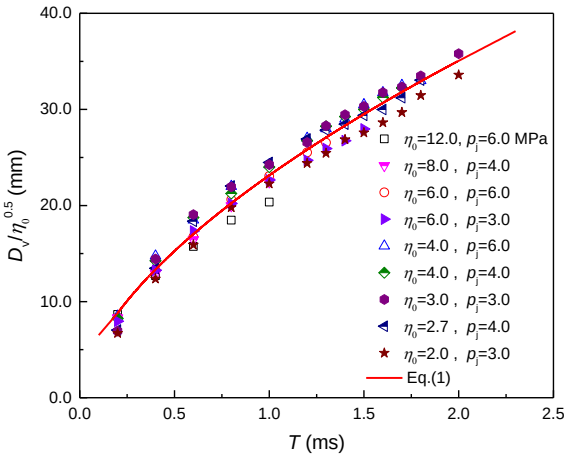


Fig 4. Diameters of growing vortex ball

The core length is a characteristics parameter to characterize the distance that pure fuel jet can travel, however, the vortex ball was used to scale the size of the zone where fuel/air is relatively well-premixed. In the present work, the measurement of the varied vortex diameter was implemented on the basis of the gaseous jets structure prediction. Nonlinear fitting was performed to explore the influences of NPR and injection time on vortex diameter. A fair correlation was achieved to estimate the diameter of H2 jet vortex, given as

$$D_v = 23.14\eta_o^{0.5}t^{0.6} \quad (1)$$

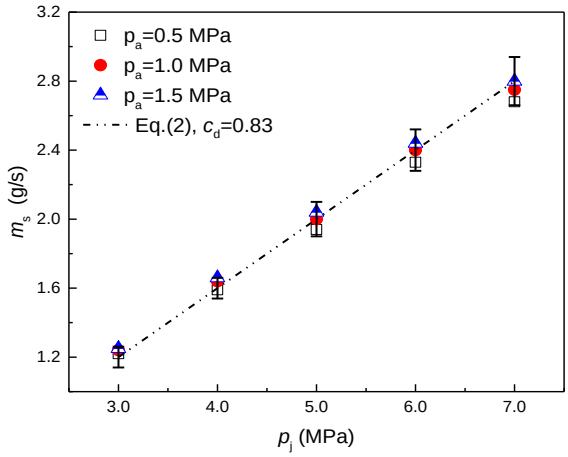


Fig 5. Steady injection rates of high-pressure hydrogen jets against injection parameters.

The total mass delivery of a H2 jet, MF, should be calculated as the sum of these above three periods of injection. However, considering the short-duration characteristic of the initializing injection and tail injection, compared to that of the stable injection, MF can be approximated as the injected fuel mass during the stable injection period. In this sense, the study on the effects of jet parameters on ms is of great significance. Fig.3 also shows that ms is a function of the jet injection parameters. The varied ms are plotted in Fig.5. It is of indicative that ms is strongly depended upon the jet pressure, while shows weak correlations against the ambient pressure. Following the isentropic analysis, the steady mass delivery rate of chocked gaseous jets can be theoretically calculated by [22]

$$m_s = c_d A_e (k\rho_j p_j)^{\frac{1}{2}} \left(\frac{2}{k+1}\right)^{\frac{k+1}{2(k-1)}} \quad (2)$$

where k , ρ_j and A_e respectively denote the adiabatic coefficient and density of the high-pressure jet, and the effective area of nozzle orifice, and c_d is the discharge coefficient, $0.0 < c_d < 1.0$. As ρ_j is linear correlated to pressure. Eq. (2) also indicates the steady fuel delivery rate, ms is linearly rated to the jet pressure, pj. Theoretical trial calculations were conducted for these jets. The results are plotted in Fig.5 as well. One can find good consistent yielded between our prediction and the formula results of $c_d = 0.83$.

4. Conclusion

High-pressure H2 jets were numerically modeled by solving K-ε model combined governing equations for gas phase flow. The transient structure and global properties of the under-expanded gaseous jets were explored, to find the key factor and quantify its influence on the micro-structures and the important global characteristic of the gaseous jets. The main conclusions were drawn as follows:

The length of the jet core presents a rapid increase and then stay at a steady value, LC. The injection pressure and the ambient pressure hardly show any direct effects on the steady core length, while a strong relationship was observed between NPR, i.e. the ratio of injection pressure to the ambient pressure, and LC. The results identify the linear dependency of LC on the nozzle diameter and the square root of NPR.

With the elapse of the injection time, the vortex ball would gradually be pushed away from the nozzle, and grows up. Following nonlinear fitting the data of vortex diameter, it is suggested that the vortex diameter is linearly increased with the square root of NPR and 0.6 power of the injection time.

The linear correlation was still observed between the non-dimensional penetration of high-pressure H2 jets and the square root of the injection time. This work presents a linear slope of about 2.7, slightly less than 3.0, the literature date.

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