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The Influence of Mixedness on Ignition for Hydrogen Direct Injection in a Constant Volume Combustion Chamber

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Abstract: The ignition behavior of the fuel in non-premixed turbulent combustion applications such as diesel engines and gas turbines is dependent on the mixing rate of the injected fuel and the working fluid. In this study, three-dimensional modeling of hydrogen injection into a constant volume combustion chamber (CVCC) is used to investigate the correlation between the mixing rate and important parameters of non-premixed combustion, such as ignition delay. Mixedness is quantified using mean spatial variation, which reflects the homogeneity of the mixture, and mean scalar dissipation, which represents the local gradients of the scalar. The case studies include nitrogen and argon as working fluids; injection velocities and nozzle diameters are varied for comparison. For consistency, the injected mass is kept constant and the injection duration is adjusted accordingly. The results indicate that a strong correlation exists between ignition delay and the defined mixedness parameters. The cases with higher mixedness values lead to a shorter ignition delay and a higher maximum flame temperature. Changing the working fluid and injection parameters can effectively modify the mixedness, and consequently affect the ignition onset and flame properties.

Keywords: Mixedness, Ignition Delay, Hydrogen Injection, CVCC

1. Introduction

Recently, hydrogen as a potential alternative fuel for use in internal combustion engines has gained interest among researchers due to its wide flammability range and the elimination of major pollutants [1]. Direct injection can be an optimal utilization of hydrogen since it removes the low hydrogen density restriction and enables a higher volumetric efficiency [2]. Moreover, it prevents backfire, which is a major problem of premixed hydrogen combustion [3]. There are a number of studies on the use of hydrogen in direct injection applications. Controlling autoignition of hydrogen in an optical engine has been investigated by attempting various injection strategies [4]. Numerical modeling has indicated that dual fuel hydrogen-diesel internal combustion engines can operate more efficiently due to the power density enhancement [5]. Adding hydrogen to natural gas-diesel engines has been observed to provide more complete combustion at low loads and a reduction of unburned hydrocarbons and CO emissions [6]. Additionally, it has been shown that hydrogen as an additive to CNG increases the maximum engine speed [7].

The fundamentals of the gaseous jet should be well understood in order to investigate the combustion characteristics of hydrogen injection. A parametric study has been carried out on high speed hydrogen injection, which shows the effect of grid resolution, Adaptive Mesh Refinement (AMR), and injection timing on mixture formation inside the cylinder [8]. The characteristics of hydrogen under-expanded jets has been comprehensively investigated using Large Eddy Simulation (LES) with different nozzle pressure ratios [9].

Replacing the working fluid can drastically impact the combustion characteristics since it can increase the ideal thermal efficiency by using high specific heat ratio gases such as argon and xenon instead of nitrogen [10, 11]. A more recent experimental study has been carried out on the effect of noble gases on fuel propagation and thermal characteristics of gaseous direct injection; it has been shown that argon can be a potentially beneficial alternative working fluid [12]. In another study, penetration length, cone angle, mixedness, and flame properties have been extensively studied for hydrogen injection into different working fluids by numerical modeling, indicating that replacing nitrogen with argon and xenon can dramatically change the jet development in the chamber [13].

One of the main properties of turbulent gaseous injection is the mixing rate of the jet with the working fluid. The mixedness of the fuel with the in-cylinder gases can heavily influence the combustion process, since ignition occurs at the smallest length scales where turbulent mixing is important [14]. However, research on quantifying the mixedness is quite limited. In one study, mean spatial variation in combination with mean scalar dissipation were used to evaluate mixedness in the turbulent injection of gasoline into air [15]. The mean spatial variation (Equation 1) represents the inhomogeneity of the scalar population, and the mean scalar dissipation (Equation 2) indicates the rate of fine-scale mixing. ζ is the conserved scalar (e. g. mixture fraction), ζ_m is the average intensity over an N by P pixel region of interest, and λ_D is the strain-limited length scale.

$$\frac{\sigma}{\xi_m} = \frac{\left\{ \left[1/(NP) \right] \sum_{i,j}^{N,P} \left[\xi_{i,j} - \xi_m \right]^2 \right\}^{1/2}}{\xi_m} \tag{1}$$

$$\chi_m = \frac{1}{NP} \sum_{i,j}^{N,P} \frac{\left(\nabla \xi_{i,j} . \nabla \xi_{i,j} \right)}{\left(\xi_m / \lambda_D \right)^2} \tag{2}$$

This method has been implemented on the direct injection of hydrogen into different working fluids, and it has been shown that argon can provide a better mixing conditions for the injected gas when compared to nitrogen due to a higher diffusivity coefficient [16]. In the present study, a three dimensional transient simulation of hydrogen injection into a constant volume combustion chamber (CVCC) is used to investigate the effect of mixedness on ignition properties.

2. Methodology

2.1 Numerical setup

Numerical simulations of hydrogen injection into a CVCC are conducted using CONVERGE computational code [17]. The CVCC is a cylindrical type with a diameter of 20 mm and a length of 50 mm. Three nozzle diameters (0.8, 1.0, and 1.2 mm), five injection velocities (80, 90, 100, 110, and 120 m/s), and two working fluids (79% nitrogen, and argon, in combination with 21% oxygen) aided to generate a sufficient number of case studies. The injection duration is adjusted based on the related velocity and diameter in order to have an equal injected mass in all the cases. A varied time step size with a minimum of 1e-7 s, and a maximum of 3e-4 s is used. CFL number, which is a vital criterion for convergence, and Mach number automatically modify the time steps. A CHEMKIN format mechanism with 10 species and 21 reactions [18] including thermodynamic data is used for the hydrogen combustion. The initial conditions inside the chamber are kept constant for all the cases at 1000 K and 1 bar, and zero heat flux boundary condition is chosen for the chamber walls. For combustion modeling, SAGE detailed chemistry solver [19], which calculates the reaction rates for each elementary reaction, is used. A 1-equation dynamic structure type of Large Eddy Simulation (LES) is implemented for turbulence modeling. CONVERGE automatically generates the computational cells, with the required base grid size set to 1 mm in this simulation. Adaptive Mesh Refinement (AMR) is utilized for the velocity and temperature with maximum embedding levels of 4 and 3 and sub-grid criterion of 0.1 m/s and 2.5 K, respectively. This method of grid refinement is quite beneficial since it generates smaller cells in high gradient areas and leads to greater computational efficiency.

2.2 Data analysis

The steepest slope of the OH radical concentration curve is used to measure the ignition delay [20]. The output image at the onset of combustion generated by CONVERGE is then exported to MATLAB for image processing. Equations 1 and 2 are then discretized and implemented on the region of interest in order to calculate the mixedness parameters.

3. Results and Discussion

Five injection velocities (V_{inj}), three injector diameters (d_{inj}), and two working fluids provide 30 different case studies which are shown in Figure 1. Blue and red dots represent nitrogen and argon, respectively, as the working fluid in combination with oxygen. A strong correlation exists between the mean spatial variation and the mean scalar dissipation. This result is in line with the previously generated plot by Probst and Ghandhi [15]. The trend line indicates that the two mixedness parameters are correlated with a quadratic function. This originates from the linear relation of spatial variation and the quadratic relation of spatial variation to the scalar magnitudes.

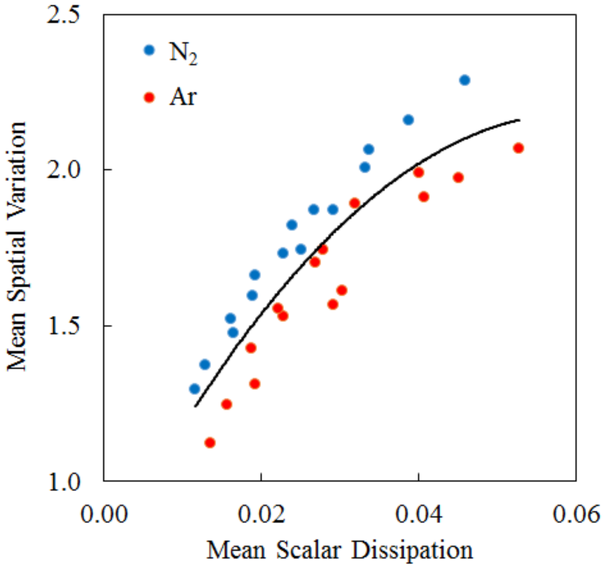

Figure 1. Mean spatial variation versus mean scalar dissipation for different working fluids, injection velocities, and injector diameters.

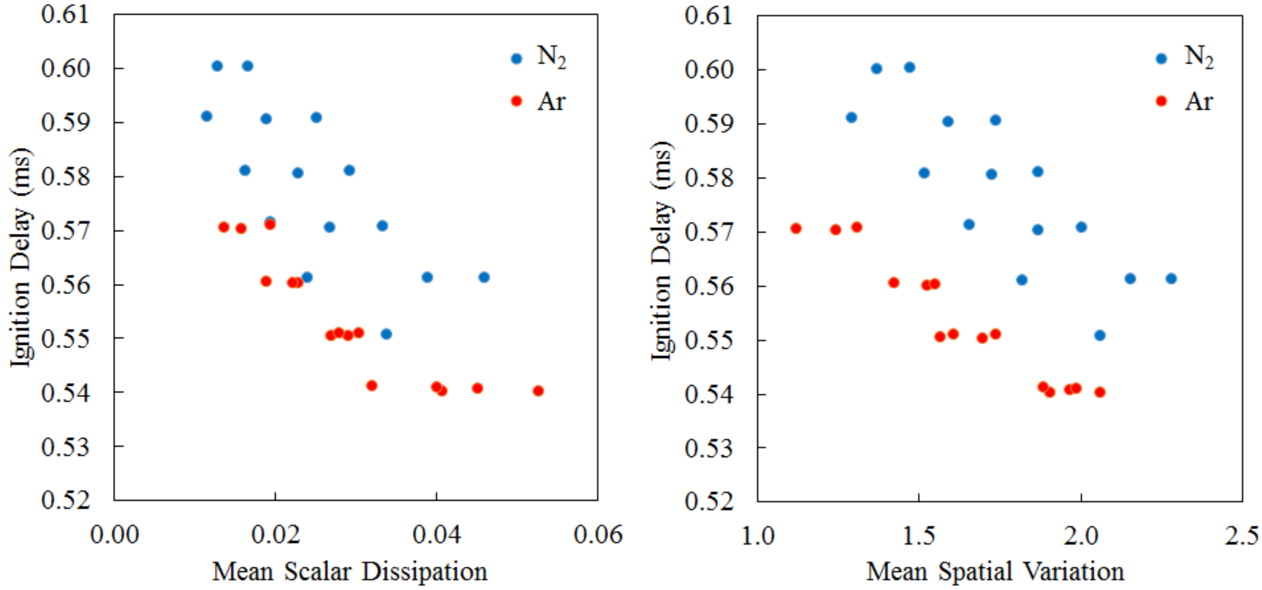

Figure 2. Ignition delay versus mixedness parameters

Figure 2 indicates the influence of the mixedness parameters on ignition delay. It can be interpreted that a higher mean scalar dissipation and a higher mean spatial variation lead to shorter ignition delay. In identical injection conditions, argon cases possess a shorter ignition delay when compared to nitrogen cases. In general, the ignition delay shows a more quadratic correlation with the mean scalar dissipation when compared to the mean spatial variation, which is more linear.

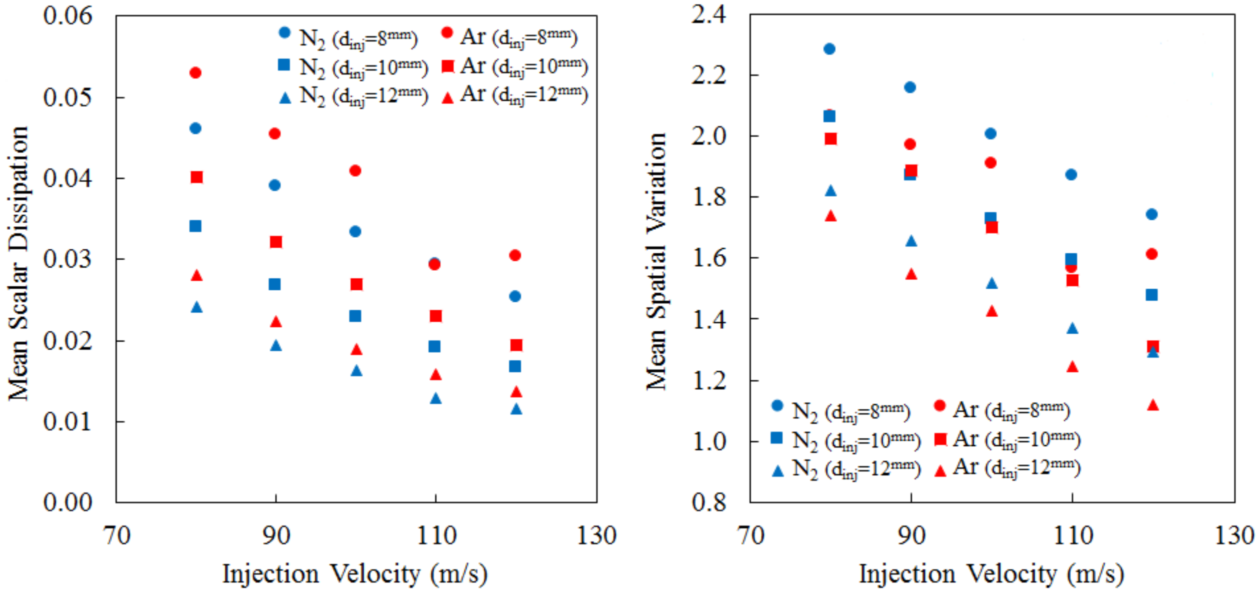

Figure 3. Effect of injection velocity and injector diameter on mixedness parameters

The effects of injection strategies on mixedness can be found in Figure 3. As seen, increasing the injection velocity can strongly affect both mixedness parameters, which affects both the ignition timing and combustion properties. Increasing the nozzle diameter has a similar effect on both the mean scalar dissipation and spatial variation. This indicates that although argon provides a shorter ignition delay in general when compared to nitrogen, changing the injection parameters such as injection velocity and nozzle diameter can drastically impact the mixedness of the injected fuel into the working fluid; therefore, hydrogen shows a shorter ignition delay in nitrogen for some cases.

Investigating the effect of other parameters in non-premixed combustion of hydrogen such as various initial temperature and pressure, and a different injected fuel temperature can help to find a more detailed correlation of the combustion properties such as ignition delay with the determinant parameters. This procedure can be implemented on other gaseous fuels such as methane, or gas mixtures (e.g. syngas) in order to provide a larger number of case studies. Providing an experimental setup can effectively aid to validate the numerical results and derive a general correlation between gaseous injection parameters and combustion properties such as ignition delay.

4. Conclusions

In this study, the effect of injection velocity, nozzle diameter, and working fluid on the mixedness parameters and ignition properties is investigated using a three dimensional transient simulation of hydrogen injection in a constant volume combustion chamber. The results indicate that increasing the injection velocity and nozzle diameter can heavily impact the mixing rate of the injected fuel and the working fluid, which dramatically change combustion properties, such as ignition delay. The relationship between two mixedness parameters, scalar dissipation and spatial variation, follow previous experimental results. The correlation of mixedness parameters to the ignition delay generated from this numerical modeling promises a potential general equation for the ignition delay calculation in all non-premixed gaseous combustion applications. An experimental study, which is currently in progress, can effectively aid to validate the modeling results and provide a comprehensive correlation for all gaseous injection cases.

5. Acknowledgements

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