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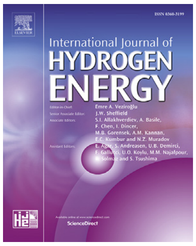

A numerical investigation of hydrogen injection into noble gas working fluids

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ABSTRACT

The thermodynamic efficiency of internal combustion engines is primarily dependent on the compression ratio and specific heat ratio of the working fluid. Due to a higher specific heat ratio, using a noble gas and oxygen instead of air can increase the thermal efficiency. The lack of nitrogen in the working fluid also eliminates NOx formation. In this study, the three-dimensional turbulent injection of hydrogen into a constant volume combustion chamber has been modeled and compared to mixtures of oxygen with nitrogen, argon, and xenon at different injection velocities. The results indicate that the hydrogen jet has a longer penetration length in nitrogen compared to argon and xenon. However, smaller penetration lengths lead to more complex jet shapes and larger cone angles. Combustion in a noble gas environment results in higher temperatures and OH radical concentrations, due in part to lower specific heats and the jet characteristics. Furthermore, mixedness is investigated using mean spatial variation and mean scalar dissipation. Hydrogen in argon shows a better mixing rate compared to nitrogen and xenon due to the higher diffusivity. The results indicate that reduction in mean spatial variation can lead to a shorter ignition delay.

Introduction

The ideal thermal efficiency of an internal combustion engine is strongly dependent on the specific heat ratio of the working fluid and the compression ratio. In compression ignition engines, the ideal thermal efficiency is calculated based on the diesel cycle formulation (Equation (1)). The cutoff ratio (α) is the ratio between the end and start volume for the combustion phase. Higher compression ratios (r) and specific heat ratios (γ) enable the thermodynamic cycle to have a higher efficiency. An increase in the ideal thermal efficiency can be achieved by replacing nitrogen with higher specific heat ratio gases such as argon and xenon. These efficiency gains have been roughly demonstrated by several groups [2,3]. Moreover, using noble gases in combination with oxygen effectively eradicates NOx from the combustion products due to the lack of ambient nitrogen [4].

$$\eta = 1 - \frac{1}{r^{\gamma-1}}\left(\frac{\alpha^{\gamma}-1}{\gamma(\alpha-1)}\right) \tag{1}$$

Although hydrogen production is still a challenge [5–8] and there are some obstacles with distribution [9,10] and storage [11,12], a broad flammability range and the elimination of major pollutants make it a potential alternative fuel for use in hydrogen fuel cell vehicles [13–15], aerospace transportation [16], and internal combustion engines [17–19].

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Nomenclature

C_L	Volume fraction constant
C_s	Smagorinsky constant
d_f	Nozzle diameter
d	Distance to the closest wall
D	Scalar diffusivity
K	Turbulence kinetic energy
L_s	Mixing length
L^*	Fine length scale
N	Number of pixels in x-axis
P	Number of pixels in y-axis
r	Compression ratio
Re	Reynolds number
S	Penetration length
$\bar{S}_{ij}$	Rate of strain tensor for the resolved scale
$\tilde{S}$	Normalized Penetration length
Sc	Schmidt number
t	Time
$\tilde{t}$	Normalized time
U_f	Injection velocity
α	Cutoff ratio
γ	Specific heat ratio
δ	Integral length scale
Δ	Length of computational cell
ε	Dissipation of turbulence energy
η	Ideal thermal efficiency
θ	Cone angle
κ	von Karman constant
λ_D	Strain-limited length scale
Λ	Scaling coefficient
μ_t	Eddy-viscosity
ν	Kinematic viscosity
ξ	Conserved scalar
ξ_m	Average conserved scalar
ρ	Density
$\tilde{\rho}$	Density ratio of fuel and working fluid
σ	Spatial variation
χ	Scalar dissipation
χ_m	Mean scalar dissipation

Direct injection can be a beneficial method to utilize hydrogen in engines, as it effectively prevents backfire [20] and increases the possibility of reaching a higher volumetric efficiency since it removes the low H_2 density restriction. There are a number of studies on hydrogen direct injection with experimental and numerical approaches. The use of hydrogen direct injection in a diesel engine has indicated that a higher power to weight ratio can be obtained compared to a conventional diesel engine [21]. In another study, direct injection of hydrogen in an internal combustion engine has been shown to effectively control the undesirable combustion of hydrogen, and enables the engine to achieve high thermal efficiency and output power [22]. To improve the overall efficiency of a hydrogen direct injection engine, a new geometry with an increased compression ratio and a longer piston stroke has been developed [23]. Using a high pressure injector for improving the efficiency and lowering the NOx productions has been experimentally investigated [24]. Controlling autoignition of hydrogen in an optical engine has been studied by attempting various injection strategies [25]. Additionally, it has been shown that hydrogen as an additive to CNG increases the maximum engine speed [26]. Numerical modeling has indicated that dual fuel hydrogen-diesel internal combustion engines can operate more efficiently due to the power density enhancement [27]. 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 [28]. The behavior of ignition delay and detonation for hydrogen combustion engines has been extensively investigated using a numerical approach [29]. In another numerical study, the mixture formation characteristics in a direct injection hydrogen engine has been studied using adaptive mesh refinement and subsonic flow assumptions [30]. The characteristics of hydrogen under-expanded jets has also been comprehensively investigated using Large Eddy Simulation (LES) with different nozzle pressure ratios [31].

However, the application of hydrogen injection into the mixture of oxygen and noble gases as working fluids, which can enhance the thermal efficiency, is not well understood. In this study, the effect of the injection velocity along with the impact of working fluid on the hydrogen jet is investigated. Important parameters include tip penetration length, cone angle, history of maximum temperature and OH mass fraction, ignition delay, and the mixing of the injected fuel with the working fluid.

Methodology

Numerical setup

A three-dimensional transient simulation of hydrogen injection into a constant volume combustion chamber (CVCC) is implemented in ANSYS Fluent. The cylindrical chamber has a 50 mm length and 20 mm diameter. The injector diameter is 1 mm. A structured mesh with increased refinement close to the centerline and the inlet is generated in order to enhance the computational efficiency. After the grid dependency test on penetration length and cone angle, a total number of 198000 cells were defined for the computational domain. The jet behavior and combustion characteristics are considered until 6 ms after the start of injection. A constant time step size of 2 μs is selected to clearly observe the jet progress and the ignition event. The density-based solver, which solves the governing equations of continuity, momentum, energy, and species transport simultaneously, is used for this simulation. For turbulence, a Large Eddy Simulation (LES) with a Smagorinsky-Lilly sub-grid scale model is applied [32]. This turbulence model is consistent with the bounded second order implicit transient formulation. The eddy-viscosity formulation (μ_t) is shown in Equation (2).

$$\mu_t = \rho L_s^2 \sqrt{2\bar{S}_{ij}\bar{S}_{ij}} \tag{2}$$

In Equation (2), L_s is the mixing length for sub-grid scales, as shown in Equation (3) where κ is the von Karman constant, d is the distance to the closest wall, C_s is the Smagorinsky

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