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# A comparative study of highly underexpanded nitrogen and hydrogen jets using large eddy simulation

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## ABSTRACT

Three-dimensional large eddy simulations (LES) of highly underexpanded hydrogen and nitrogen jets at the same nozzle pressure ratio (NPR) of 5.60 and at a Reynolds number around  $10^5$  are performed. The classical near-field structures of highly underexpanded jets are well captured by LES, especially the shape and size of Mach barrel for both jets are very similar and agree well with the available literature data. However, the flow field and the shock structures after the Mach disk differ significantly. The density in the annular shear layer of  $H_2$  jet is much lower because of its smaller molecular weight. Meanwhile, the  $H_2$  jet has a much longer jet core and more shock cells. The dominant instability mode is helical for the  $N_2$  jet, but is axisymmetric for the  $H_2$  jet. There are two discrete peaks of  $f_s = 37.086$  kHz and  $f_{2s} = 45.695$  kHz in the spectrum of the  $N_2$  jet, while the spectrum of the  $H_2$  jet is characterized by a fundamental screech frequency of  $f_s = 47.020$  kHz and its high-order harmonics. The  $H_2$  jet mixes more rapidly with the ambient air but has a much smaller mixing area on cross-section planes. Mixing between the ambient air and fuel still takes places at the jet boundary defined according to the mixture fraction of  $Z = 0.02$ , and the area of fully turbulent region of the highly underexpanded jets seems to be less predicted based on the traditional vorticity  $T/NT$  (turbulent/non-turbulent) interface for both jets.

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## Introduction

Scramjet engine is one of the most promising propulsive systems for future hypersonic vehicles because of its high performance at large Mach number. Usually air entering the combustor is supersonic at flight speeds beyond Mach 5, thus the residence time of the air in a scramjet engine is on the order of milliseconds [1]. The mixing and diffusive

combustion of fuel and air in a conventional scramjet engine take place simultaneously in the combustor. Therefore, ensuring fuel-air mixing and subsequently combustion in such a short time is critical to the design of scramjet engine [2–4].

In spite of the high price in production and storage, hydrogen is a very attractive fuel that may help to resolve the problem because of its higher combustion efficiency than conventional hydrocarbon fuels. Hydrogen gives the highest

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heat release with the shortest kinetic time [5,6], and is already used as fuel in space propulsion [7,8]. In addition, hydrogen is generally considered to be more environment-friendly since it does not produce any harmful pollutants like carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), or particulate matter during the combustion process except the minor NO<sub>x</sub> formation due to its high-adiabatic flame temperatures. The fuel is usually injected into the combustor at a pressure much higher than the ambient pressure to ensure a good mixing, which will result in a highly underexpanded jet [9–12]. For the design benefit, revealing the flow characteristics and understanding the physical mechanism of a highly underexpanded hydrogen jet are conducive to the development of scramjet engine.

The highly underexpanded jet is characterized by the presence of a Mach disk in the near-field region and defined by a nozzle pressure ratio (NPR) beyond 3.85 [12]. Adamson and Nicholls (1959) [9] presented the structure of a highly underexpanded jet into quiescent air firstly. Ashkenas and Sherman (1965) [10] indicated that the near-field structures of highly underexpanded jets are dominated by NPR and obtained an empirical formula to predict the Mach disk height according to NPR. Over the years, several more experimental [11–19] and numerical [20–24] studies have been conducted, which have resulted in a good understanding of the flow characteristics of highly underexpanded jets today. One may refer to the recent review of Franquet et al. (2015) [25] for further details. However, the knowledge on a highly underexpanded hydrogen jet is still limited since most of the injected gases used in previous studies are air or nitrogen. Hydrogen has higher diffusivity and larger nozzle exit speed due to its low molecular weight, which may result in a much different flow field even at the same NPR. In addition, the previous experimental and numerical studies on highly underexpanded jets mainly provide the time-averaged flow characteristics in the near-field region of jets by using schlieren photographs and Reynolds averaged Navier–Stokes (RANS) methodology respectively. The instantaneous unsteady flow features of a highly underexpanded jet that dominate the mixing processes are still not well revealed.

Large eddy simulation (LES), which resolves the large scales directly while models the effects of small scales, is turbulence-well-represented yet computationally affordable for the simulation of supersonic shear flows with high compressibility. In recent years, LES researches [26–30] on underexpanded jets have emerged thanks to the advances in numerical methods and computation technology. In particular, Gorle et al. (2010) [28] conducted a computational study of highly underexpanded hydrogen jet at NPR = 30.0, and found that the near-field structures captured by the LES have a good agreement with the experiments. However, their main goal was to verify the jet injection modeling and an in-depth analysis on the instantaneous flow features was not performed. Recently, Hamzehloo and Aleiferis (2015) [30] performed a numerical analysis of underexpanded hydrogen jets with different NPRs using LES, where the transient flow development upstream of the nozzle exit was investigated, as well as the effect of NPR on the mixing characteristics and near nozzle shock structures were analyzed. Besides the near-field shock structures, screech tone of underexpanded supersonic jets is another important subject of many experimental and theoretical studies [26,27,31–36] since its first experimentally

observation by Powell (1953) [31]. However, the working gases are usually air/nitrogen as well in those studies, whereas the data on the screech characteristics of highly underexpanded hydrogen jets are rather lacking in the literature.

In the present study, a three-dimensional LES of high pressure hydrogen jet through a convergent nozzle with an exit diameter of  $D = 2.0$  mm and an exit Reynolds number around  $10^5$  was carried out. A test case of nitrogen injection at the same NPR of 5.60 was also simulated for comparison. A well-designed, hexahedral and block-structured grid containing about 27.3 M computational cells is applied. The compressible flow solver, astroFoam, which is developed based on the OpenFOAM C++ library, is used to perform the simulations. The time evolution, averaged jet structures, shock structures, dominant instability modes, and mixing characteristics of the H<sub>2</sub> jet are analyzed and discussed in comparison with the N<sub>2</sub> jet.

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## Computational methodology

Three-dimensional, Favre-filtered Navier–Stokes equations for the unsteady compressible Newtonian fluids with heat and species transfer are solved using a density-based compressible solver, astroFoam, which is developed based on the standard rhoCentralFoam solver distributed with OpenFOAM v2.3.0. The rhoCentralFoam solver [37] has been proved to be able to capture the flow discontinuities (e.g. shock waves) with non-oscillatory and low dissipation by solving the convection-diffusion equation using the semi-discrete K-T central scheme [38]. However, the rhoCentralFoam solver is limited to single species non-reacting flows in its standard form. The multiple species transport and multi-component diffusion are added to create the astroFoam solver to investigate the gases mixing and reacting flow. In addition, the astroFoam solver solves for sensible enthalpy equation instead of the transport of total energy in rhoCentralFoam solver in order to easily include the chemical reaction and species transport terms. Similar OpenFOAM solvers have been developed to study the incompressible turbulent flows by Vuorinen et al. (2011) [39] and Baba and Tabor (2009) [40] as well as the supersonic compressible turbulent flows by Vuorinen et al. (2013) [29] and Fureby et al. (2011, 2013) [41,42]. The filtered sub-grid terms are modeled with the sub-grid scale turbulent kinetic energy one-equation model, which is integrated in OpenFOAM in the standard form.

## Computational domain and grid

Previous studies [31–36] indicated that the sound waves originated in the downstream will propagate upstream to change the initial shear layer structures at the nozzle exit, which will influence the development of jet shear layer in the downstream further. However, A priori knowledge of nozzle exit conditions is usually difficult to be obtained in many practical applications. Therefore, the numerical investigation of underexpanded jets requires implementing the practical nozzle geometries to capture the self-sustained acoustic loop correctly. Some example of such endeavors can be found in

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