Modeling of non-premixed hydrogen jet combustion in an argon/oxygen environment via direct and Reynold's averaged numerical simulations

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Abstract

The Argon Power Cycle (APC) is a highly efficient, emission-free energy conversion system. The APC considered in this study burns hydrogen and oxygen in an argon environment using a direct-injected (DI) compression-ignition (CI) engine. The combustion process of the DI-CI APC, as well as of air-breathing DI-CI hydrogen engines, is predominantly non-premixed. The development of such engines requires the use of models, such as Reynolds Averaged Navier Stokes (RANS). In practice, commercial, low-order software code is often used. This work assesses the adequacy of the widely used software package CONVERGE employing RANS combined with a detailed chemistry combustion model by comparing simulation results of a turbulent, igniting planar hydrogen jet with a direct numerical simulation. The results show that mass and momentum transport is predicted satisfactorily. Larger differences were found in temperature and species mass fraction profiles, which can be attributed to the absence of turbulence-chemistry interaction. This work contributes to the development of accurate and computationally efficient numerical models to simulate diffusive hydrogen jet flames.

Keyword: DNS, RANS, hydrogen, jet, non-premixed, combustion

1. Introduction

The Argon Power Cycle (APC) is a highly efficient, emission-free energy conversion system [1, 2] that can help solve the problem of intermittent energy supply from renewable sources. The APC considered in this study represents one based on hydrogen and oxygen combustion in an argon environment, using a Direct-Injection (DI) Compression-Ignition (CI) Internal Combustion Engine (ICE). The DI-CI APC, as well as air-breathing DI-CI hydrogen engines, require the hydrogen to be injected at high pressure, late in the compression stroke, where the temperature and pressure in the combustion chamber can reach values up to 1400 K and 140 bar, resulting in a very short ignition delay time.

To develop such engines, accurate and computationally efficient models are needed to gain detailed insights into the combustion phenomena and to reduce expensive prototyping. Adequate simulation of global in-cylinder variables, such as pressure, temperature, and heat release rate as a function of time, is crucial to predicting engine performance indicators, such as thermal efficiency and heat loss. The fuel jet can reach Reynolds numbers $Re > 10^6$. Modeling of such phenomena requires the use of statistical approaches e.g., Reynolds Averaged Navier Stokes (RANS), since resolving all scales via Direct Numerical Simulations (DNS) is computationally unfeasible. Such strategies rely on closure models whose applicability to hydrogen is not ensured, since hydrogen's physical properties largely differ from other commonly used fuels.

In practice, commercial solvers are often employed to perform such engine-scale simulations. These solvers have a bias to compute convergent solutions. This might rely on the use of low-order numerical schemes, or simplistic approximations of complex phenomena, like combustion. A widely used, commercial software package to develop ICEs, gas turbines, and other combustion applications is CONVERGE [3]. This software is used to perform the RANS simulations in the presented work. In previous work [4], we compared three-dimensional DNS with RANS simulations using CONVERGE of inert temporal mixing layers at Reynolds numbers 5,000 and 10,000 to test the validity of the RANS turbulence model. Reasonable agreement was found on mean flow properties, such as mean velocity and mean mixture fraction evolution.



Fig. 1: Schematic of the simulated periodic planar jet configuration.

In this work, we compare turbulent, reacting planar jets and focus on the combustion process to assess the adequacy of the RANS simulation for auto-igniting hydrogen jets. We show volume-integrated and spatially averaged profiles of parameters that characterize the combustion process. Finally, recommendations are made for engine-scale simulations of non-premixed hydrogen combustion. This work contributes to the development of accurate and computationally efficient numerical models to simulate diffusive hydrogen jet flames.

In the next section, the test setup to represent a $DI-H_2$ event is explained and details of the two computational fluid dynamics codes are provided. In Sec. 3, the results of the performed simulations are discussed. Lastly, conclusions are drawn and recommendations are made in Sec. 4.

2. Numerical setups

A representative domain of DI-H₂ is defined as depicted in Fig. 1. It consists of a rectangular jet of pure H₂ at 300 K of height H = 2 mm and a mean speed $U = 565 \text{ m s}^{-1}$ surrounded by a homogeneous mixture of oxygen and argon (molar ratio 1:9) at a 1300 K and 1 bar. Effects of high pressure are not investigated here and should be done elsewhere.

2.1. DNS setup

The DNS is performed using an in-house, fully compressible solver, employing a compact finite difference scheme with sixth-order accuracy in space and third-order accuracy in time [5], named Disco. The chemical source terms are computed with the detailed chemical mechanism derived by Burke et al. [6] with 9 species and 21 reactions. Turbulence is initialized using a filtered random field of fluctuations, with a rootmean-square value of 10% of the jet speed. Navier-Stokes characteristic boundary conditions (NSCBC) [7] are used on the top and bottom planes, including transverse and other terms [8]. The other boundaries are periodic. Details on the initialization, grid size and jet velocity are given in [9]. In the DNS presented here, the domain is extended in the y-direction at $t^* = t/t_j = 50$ with $t_j = H/U$ the jet time, and the initial grid size $(dx = 12.5 \,\mu\text{m})$ is coarsened by a factor two, always ensuring that the Kolmogorov scale (η) is well resolved $(dx/\eta < 2)$.

2.2. RANS setup

The RANS simulations are performed using the commercial software package CONVERGE version 3.0 [3], employing the Renormalization Group (RNG) variant of the k- ε family developed by Yakhot and Orszag [10] with the standard values for the model constants. The compressible RANS equations are solved using the finite volume method with the density-based Pressure-Implicit Splitting of Operators (PISO) method of Issa [11]. The equations are discretized employing a flux blending scheme which is second or first-order accurate in space, depending on the local monotonicity of the flow. Time integration is performed with a first-order implicit Euler approach. A variable time-step algorithm is used to limit the Courant-Friedrichs-Lewis number to 0.4. The maximum time-step was set to 0.1 µs. The turbulent Schmidt and Prandtl numbers are both set to 0.7. Combustion is modeled with the SAGE detailed chemical kinetics solver [12], employing



Fig. 2: Evolution of T at $t^* = \{0, 20, 40, 60, 80, 100\}$ of the DNS result. The white isocontour denotes the stoichiometric mixture fraction.

the same reaction mechanism as the DNS. It is important to note that turbulence-chemistry interaction is not included in the SAGE model.

The computational domain is initialized with the Favre-averaged profiles of all required field variables (except for pressure, which is ensemble averaged) and species mass fractions of the DNS setup. Similar to the DNS setup, the left and right planes are periodic, and outflow NSCBC are applied to the top and bottom boundaries. However, the front and back planes are constrained with symmetry instead of periodic boundaries due to practical limitations. Rectangular cell elements are used, with a grid size of 0.4 mm in *y*-direction, and 0.8 mm in the other directions.

3. Results

Before comparing the RANS to the DNS results, a brief overview of the simulated process is provided using the DNS results. Figure 2 shows its time-evolution of the instantaneous temperature in an x, y plane. During the first 20 jet times, the turbulent hydrogen jet mixes with the hot, quiescent ambient. At 40 jet times, multiple ignition kernels are visible. These grow and merge until a diffusive flame front establishes around the jet at 60 jet times.

In Fig. 3, we show volume-integrated water production rates computed with RANS and DNS. This property is closely related to the heat release rate, which is arguably the most important parameter for the engine's efficiency. From the water production rate, it is observed that the DNS ignites approximately at 25 jet times. At about 45 jet times, it reaches its peak water production, indicating that the jet has ignited completely and a diffusive flame has established around the hydrogen jet.

The RANS simulation which started from an averaged DNS field at $t^* = 0$, is shown in blue. It shows that it ignites at around 40 jet times, which is significantly later than the DNS result. Consequently, the amount of fuel and oxidizer that have mixed and are available for premixed combustion is larger, resulting in a larger premixed combustion peak. Although the main trend of the DNS is captured by the RANS, the result is quite far off. The reason behind this could be the nature of the transition to turbulence, which begins with the creation of a small number of Kelvin-Helmholtz instabilities, which break up chaotically. In other words, there is a transitional phenomenon where turbulent kinetic energy is created. No mechanism that can capture this transition is present in the RANS model.

At engine conditions, the ignition delay time is very short relative to the injection duration and almost all heat will be released after a diffusive flame front has established around the jet [13]. To assess the adequacy of the RANS setup to model this non-premixed hydrogen combustion phase, we initialized the RANS simulation with the averaged field variables of the DNS corresponding to 25 jet times, which is just before ignition. At this time, the mass fractions of the reactants have partially mixed but did not react significantly. Furthermore, as the igniting kernels in Fig. 2 indicate, the reaction is not uniformly taking place, hence the concentration of radicals and reaction zones is very far from the mean profile, and comparing these dispersed phenomena to an average profile will show large deviations.

In other words, when initializing the RANS using the averaged DNS fields at jet times later than 0, an inconsistency is introduced in the two simulations. Due to spatial fluctuations present in the DNS, the averaged profiles as a function of y-coordinate do not satisfy the equation of state at each point. This means



Fig. 3: Volume-integrated net H₂O production plotted against dimensionless time.



Fig. 4: Profiles of mixture fraction, Z, and normalized streamwise velocity u plotted against normalized y-coordinate at different jet times.

that, if the RANS is initialized using averaged pressure, temperature, and species mass fraction profiles, the density profile computed from the gas law is not the same as the averaged density profile of the DNS as will be shown later.

The water production rate of the RANS simulation starting at $t^* = 25$ is shown in Fig. 3 by the solid orange line. Ignition occurs around 5 jet times after the start of the simulation, but the overall trend is captured reasonably well. To compensate for the deviation in ignition timing and to be able to better compare the DNS and RANS results, the RANS water production curve is advanced 5 jet times (dashed orange line). It shows that it can accurately capture the first part of the combustion, up to 50 jet times. Afterward, the water production is overestimated, this could be because the RANS is not able to capture turbulence chemistry interaction. As it was shown in [9], this case exhibits extinction in the fuel-side of the jet, which is not captured by the RANS. In the remainder of this paper, the results of the RANS started at $t^* = 25$ (not time-shifted) are shown.

Figure 4 shows mixture fraction and streamwise velocity profiles plotted against normalized y-coordinate. There is reasonable agreement in mixture fraction, although the RANS is slightly less dissipative at the later times. The velocity profiles compare well in both shape and magnitude. Overall, the mean mass and momentum transport is predicted adequately.

The spatial distribution of H₂ is predicted reasonably well, but less accurately compared to Z and u, see the left plot of Fig. 5. At $t^* = \{60, 80\}$, the RANS predicts lower hydrogen mass fraction at the side of



Fig. 5: Profiles of H_2 and H mass fraction plotted against normalized y-coordinate at different jet times.



Fig. 6: Profiles of temperature and density plotted against normalized y-coordinate at different jet times.

the jet. Although a similar observation is made for the mixture fraction profiles, the differences are more pronounced for the H_2 profiles. It indicates that mean reaction rates are higher in the RANS, which is also illustrated by the H profiles shown in the right plot of Fig. 5. The RANS simulation produces much higher levels of H radical at the later jet times, but the DNS shows more dispersed profiles.

The more intense combustion of the RANS is further demonstrated by the temperature profiles shown in Fig. 6. Similar to the H mass fraction profiles, the RANS profiles are less dispersed and reach higher maximum values, thereby showing a more intense and localized combustion. Lastly, density profiles are provided in the right plot of Fig. 6. The earlier explained mismatch in initial RANS density profile can be observed at $t^* = 25$. Despite this, the trends at $t^* = \{60, 80\}$ are captured reasonably well. Similar to the temperature profiles, the main differences are found at the outer side of the jet. The more localized combustion causes a large density gradient at that location. As mentioned earlier, this behavior could be caused by the absence of turbulence-chemistry interaction in the combustion model.

4. Conclusions

In this study, we performed computational fluid dynamics simulations of auto-igniting planar hydrogen jets using a high-order DNS code and a widely used commercial, low-order RANS code to validate the combustion model of the latter.

When started from the fully unmixed situation at $t^* = 0$, the RANS over-predicts the ignition delay time and consequently the premixed peak. When starting the RANS just before ignition ($t^* = 25$), the water production rate is in good agreement during the premixed combustion phase. However, during the

diffusive combustion phase, it was over-estimated. In an engine, this translates to a shorter combustion process, resulting in an over-estimated thermal efficiency (due to a better approximation of the theoretical Otto-cycle efficiency).

The above mentioned differences could be attributed to the lack of turbulence-chemistry interaction model in the RANS, which is unable to capture the spatial fluctuations of the composition in the homogeneous directions x and y. Also the higher values observed in temperature and H mass fraction profiles can be related to this. It is recommended for subsequent studies to explore combustion models in CONVERGE that include turbulence-chemistry interaction.

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