Efficient Computational Methods for Turbulent Boundary-layer H2-air Flashback Prediction

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EFFICIENT COMPUTATIONAL METHODS FOR TURBULENT BOUNDARY-LAYER H_2-AIR FLASHBACK PREDICTION

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Summary The current computational work aims to quantitatively understand the flashback phenomena to validate a practical gas turbine combustor for flexible fuel operation from 100% Natural Gas to 100% H_2 and any mixture thereof at a low emissions level. Generally, the past studies have extensively used the two configurations to study flashback, namely, jet premixed flames and divergent channel. This current study contains computational results using detailed kinetics for jet premixed H_2-air premixed flames to predict flashback. The study highlights the importance of grid sizes for accurately capturing the net hydrogen reaction rates for predicting flashback.

INTRODUCTION

Hydrogen is considered a clean alternative fuel with zero carbon emissions. Thus, a gas turbine combustion system operating on either partial or 100 % hydrogen as a fuel offers a low carbon emission solution for the energy sector. Figure 1 shows one such design for FlameSheet^{TM} combustion system by Thomassen Energy retrofitted for the High Hydrogen Gas Turbine Retrofit Project.

However, hydrogen as a fuel in gas turbine combustors also poses a challenge on the stable operation of the gas turbine combustor. Hydrogen flames are highly reactive (≈5 to 6 times) in comparison to natural gas. They are prone to flashbacks, posing a challenge for their partial to 100 % hydrogen use in gas turbine combustors. During the flame flashback in gas turbine combustors, the hydrogen flame travels upstream in the gas turbine combustor to the mixing chamber, developing a diffusion flame instead of a premixed flame. This leads to a high temperature in the mixing chamber, resulting in permanent damage to the combustor. Elbe & Mentser (1945) were the first to experimentally study the boundary layer flashback of laminar H_2-air flames using a jet flame burner setup. They developed a simple semi-empirical correlation between boundary-velocity gradient, burning velocity and tube diameter for the flashback. The current study performs detailed numerical simulations on this available experimental data to find the best computational methodology to predict H_2-air flashback. These databases will be further used for the development/validation of the efficient computational reduction methods for hydrogen combustion in gas turbine combustors using reduced kinetics and Flamelet generated manifolds methods, FGMs.

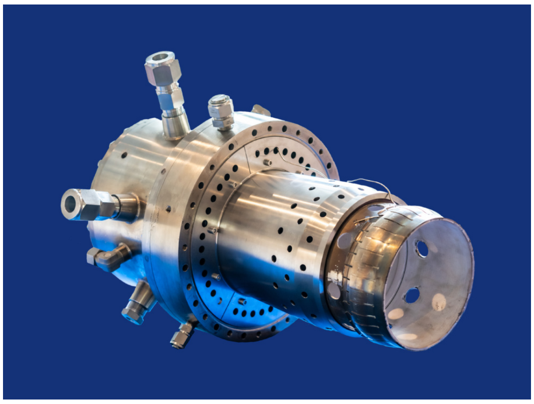

Figure 1: Design of FlameSheetTM combustion system by Thomassen Energy retrofitted for High Hydrogen Gas Turbine Retrofit Project [1]

COMPUTATIONAL METHODOLOGY

Figure 2 shows the schematic of the computational domain with imposed boundary conditions. 2D axisymmetric steady-state computations were performed using commercially available Ansys-Fluent package.

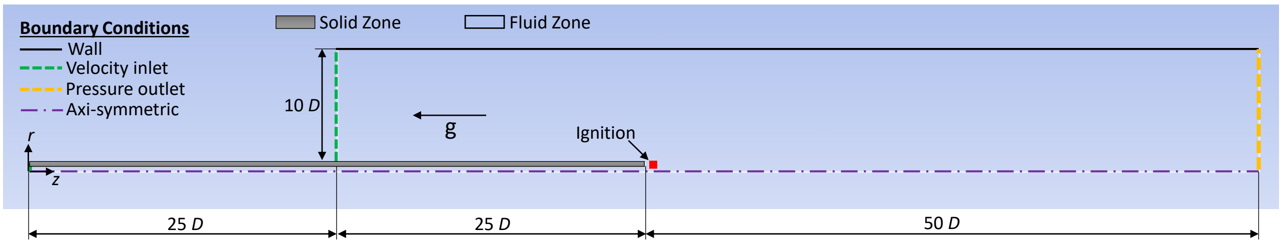

Figure 2: Schematic of the computational domain with imposed boundary conditions

Choice of jet burner diameter (D = 2.16mm) comes from Elbe & Mentser (1945) H_2-air flashback experimental data. Reactant mixtures of H_2-air were provided from the inlet ($\phi = 0.42$). Simulations were performed using Konnov (2019) H_2 oxidation kinetics mechanism. Thermo-physical properties were calculated using the kinetic theory of gases with thermal diffusion included. Conjugate heat transfer equations were solved in solid-fluid interfaces. The converged solution was obtained for an inlet velocity at which a definite stable flame solution exits (generally 1.25 times the stretch free laminar flame speed for a given H_2-air mixture). Then the reactant velocity was decreased in steps of 5-10 cm/s to obtain the flashback condition. Close to flashback condition, the velocity reduction step-size was further reduced to 2 cm/s.

RESULTS AND DISCUSSION

Figure 3 shows the variation of axial flame temperature for four grid sizes for lean mixture (ϕ = 0.42) for D = 2.16 mm at average velocity (u_{av}) of 0.7 m/s. Comparison of temperature profile shows a difference of less than 20 K when the grid is refined from 200 to 25 μm. There is no change in axial velocity profile with mesh size reduction from 200 to 25 μm (see Fig. 3 below for details).

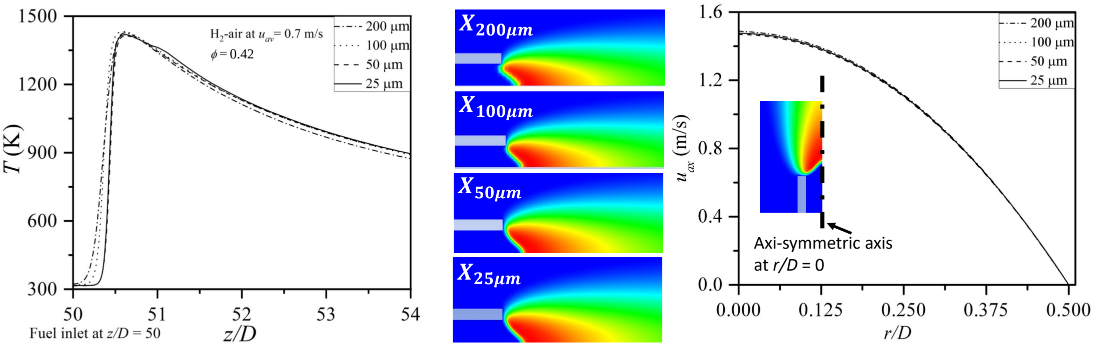

Figure 3: Variation of axial flame temperature and radial velocity for four grid sizes

Significant change is observed in the inlet velocity for the flashback conditions from coarse to refined mesh. Hence, accurately capturing the H_2 reaction rate should be the critical factor to predict flashback of premixed H_2-air mixtures (see Fig. 4). These findings are in line with the grid independence study of Ali and Varunkumar (2020) for predicting the extinction of CO/H_2 non-premixed flames.

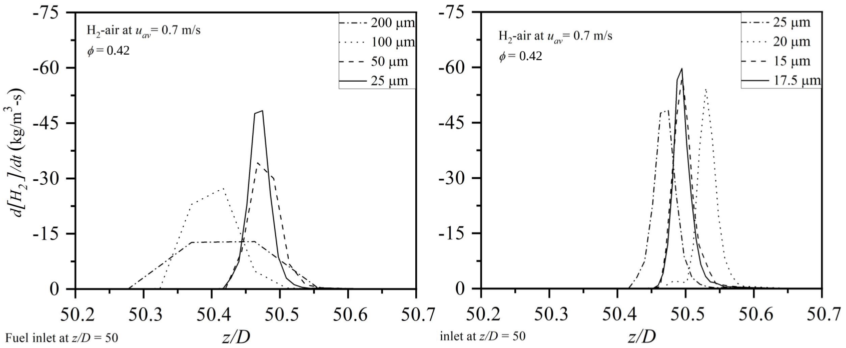

Figure 4: Variation of net H_2 reaction rate along the axis for eight grid sizes

The data shows that the flame thickness changes from 600 to 200 μm with mesh refinement from 200 to 15 μm for ϕ = 0.42. The location of H_2 reaction rate peak shifts upstream ($\approx$ 150 μm) with mesh size reduction from 25 to 20 μm with 12 % increase in peak heat release rate. The flame location does not show any change and less than 3.5 % increase in peak value for further reduction in grid size from 17.5 to 15 μm. Therefore, 17.5 μm grid size should be used to predict flashback for ϕ = 0.42 in the case of detailed kinetics simulations.

CONCLUSIONS

Mesh refinement from 200 to 25 μm shows no change in the axial velocity profile. So, the grid size that can accurately capture the H_2 reaction rate should be used to predict flashback in detailed kinetics simulations (for instance, DNS for turbulent cases). Even though the critical velocity gradient (flashback limit) does not show any significant change for the studied H_2-air lean case (ϕ = 0.42) with a grid size reduction from 50 and 25 μm, these mesh sizes cannot be recommended as a conclusive grid size for higher values of equivalence ratios. A coarse mesh size close to flame thickness is recommended in cases where reaction rates are calculated using subgrid modelling methods (FGM).

Acknowledgments

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