Preliminary results for flashback prediction in laminar H2-air premixed flames

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Abstract: The current study contains preliminary computational results using detailed kinetics for exploring the best computational methodology to **predict H_2-air flashback**. These databases will be further used for the development/validation of efficient computational reduction methods for hydrogen combustion in gas turbine combustors using reduced kinetics or Flamelet generated manifolds methods, FGMs.

1 Introduction and background information

INTRODUCTION

- H_2 is a clean alternative fuel with zero carbon emissions.
- Good alternative for gas-turbines.
- In Figure 1 our situation under investigation is displayed.

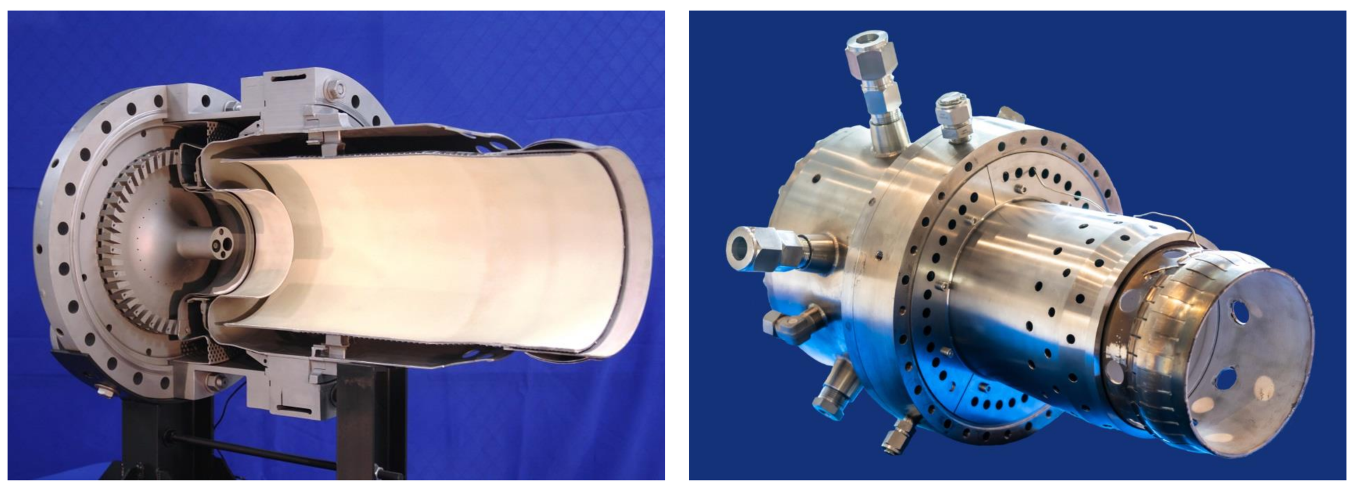


Fig. 1 Design of FlameSheet™ combustion system by Thomassen Energy retrofitted for High Hydrogen Gas Turbine Retrofit Project [1]

CHALLENGE

- Flame flashback

APPROACH

- Validation of laminar cases first.
- Based on Lewis and von Elbe (1943) theory (boundary layer gradient, burning velocity & tube diameter).
- H_2 oxidation kinetics mechanism.
- Kinetic reduction methods.
- Reduced kinetics or Flamelet generated manifolds methods, FGMs

2 Computational methodology

- 2D axisymmetric steady-state .
- Diameter (D = 2.16 mm) as in *Elbe & Mentser* [2].
- Premixed, 15/85-45/55 % (v/v) H_2/Air.
- *Konnov (2019)* mechanism used.
- Properties based on kinetic theory and conjugate heat transfer included.
- Velocities decreased from 0.7 m/s with steps of 0.05 m/s, close to flashback with steps of 0.02 m/s.

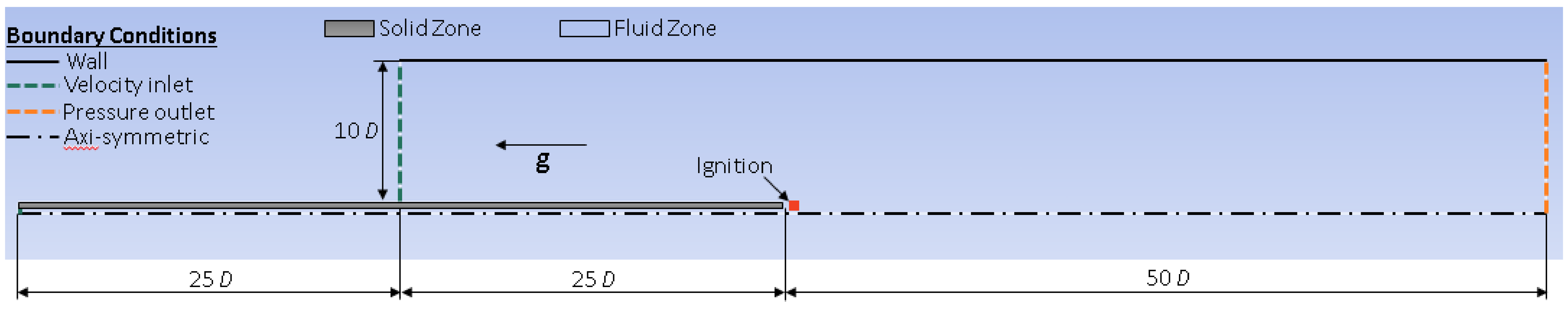


Fig. 2 Schematic of the computational domain with imposed boundary conditions

Grid Independence study

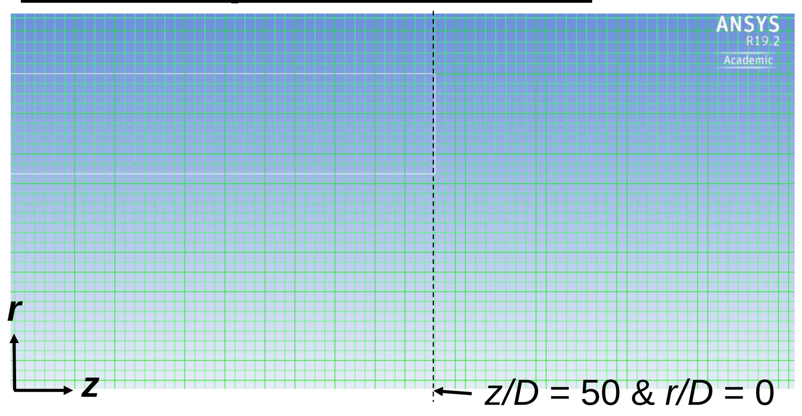
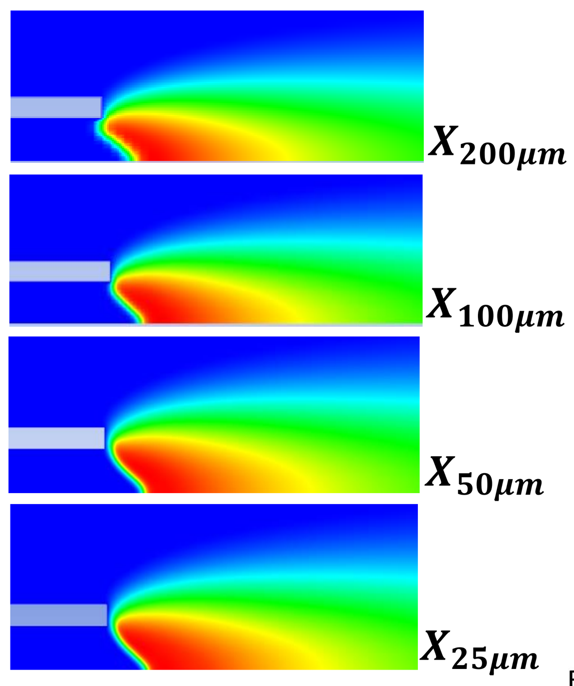


Fig. 3 Details of the computational grid used for computations.

- Uniform grid ($X_{***\mu m}$) along axial direction from z/D = 47.5-52.5
- Uniform grid along the radial direction from r/D = 0-0.75



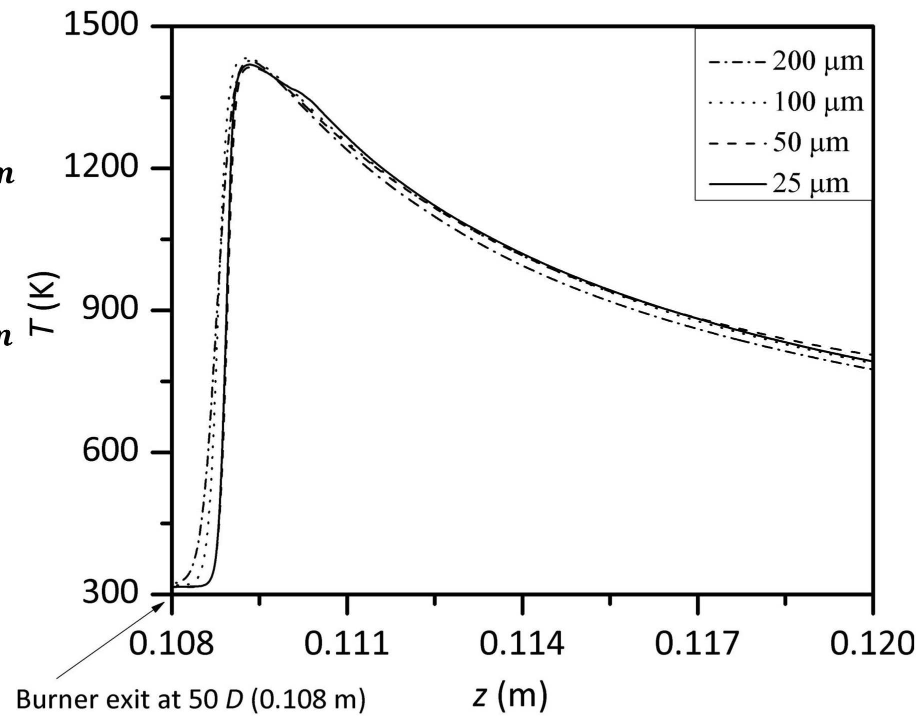


Fig. 4 Variation of axial flame temperature for four grid sizes for lean mixture containing 15 % H_2 (v/v) for D = 2.16 mm at average velocity of 0.7 m/s

- Comparison of temperature profile shows a difference of less than 20 K when the grid is refined from 200 to 25 μm.

3 Results and discussions

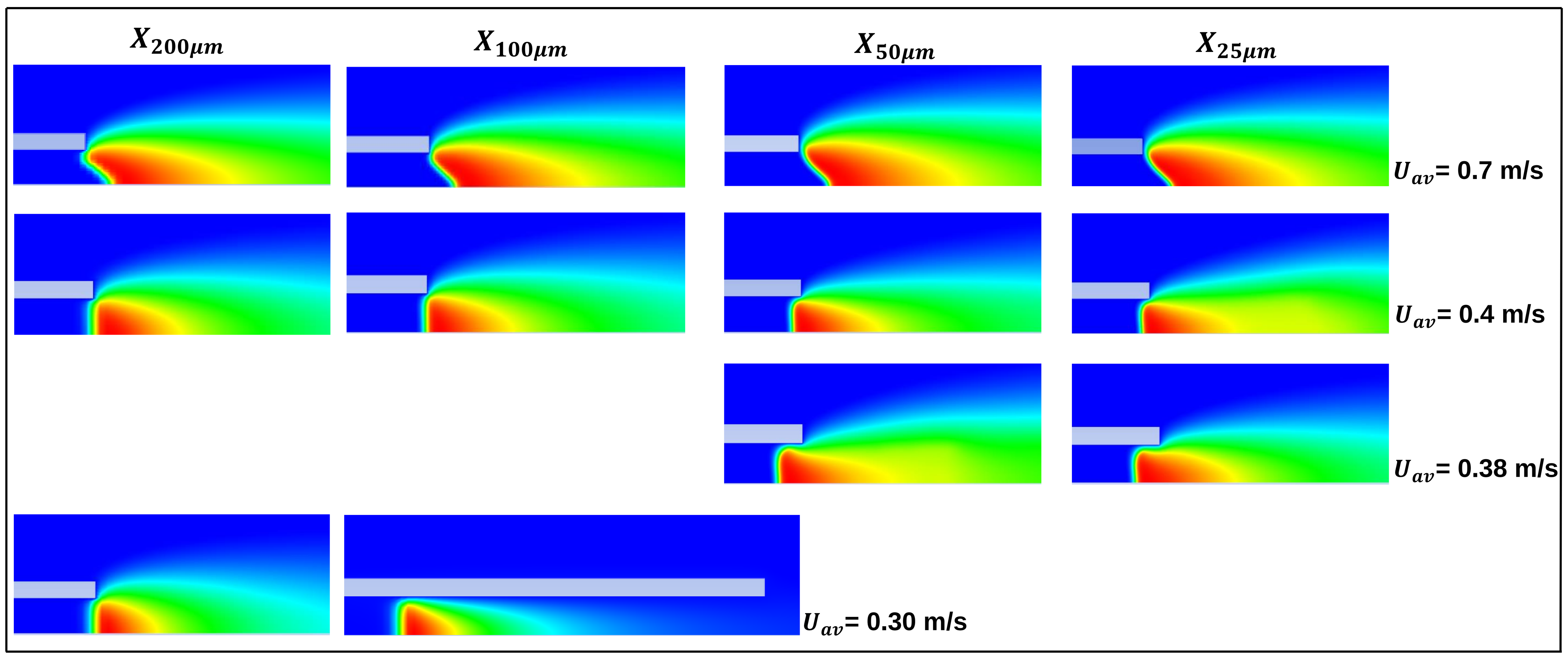


Fig. 5 Temperature profiles for Lean mixture containing 15 % H_2 (v/v) for burner diameter of D = 2.16 mm at decreasing average velocities

- Significant change is observed in the inlet velocity for the flashback conditions from coarse to refined mesh (see Figs. 5 and 6). There is no change in axial velocity profile with mesh size reduction from 200 to 25 μm (see Fig. 7). Hence, capturing the H_2 reaction rate accurately should be the key factor to predict flashback of premixed H_2-air mixtures (see Fig. 8). These findings are in line with the grid independence study of *Ali and Varunkumar (2020)* for predicting extinction of CO/H_2 non-premixed flames.

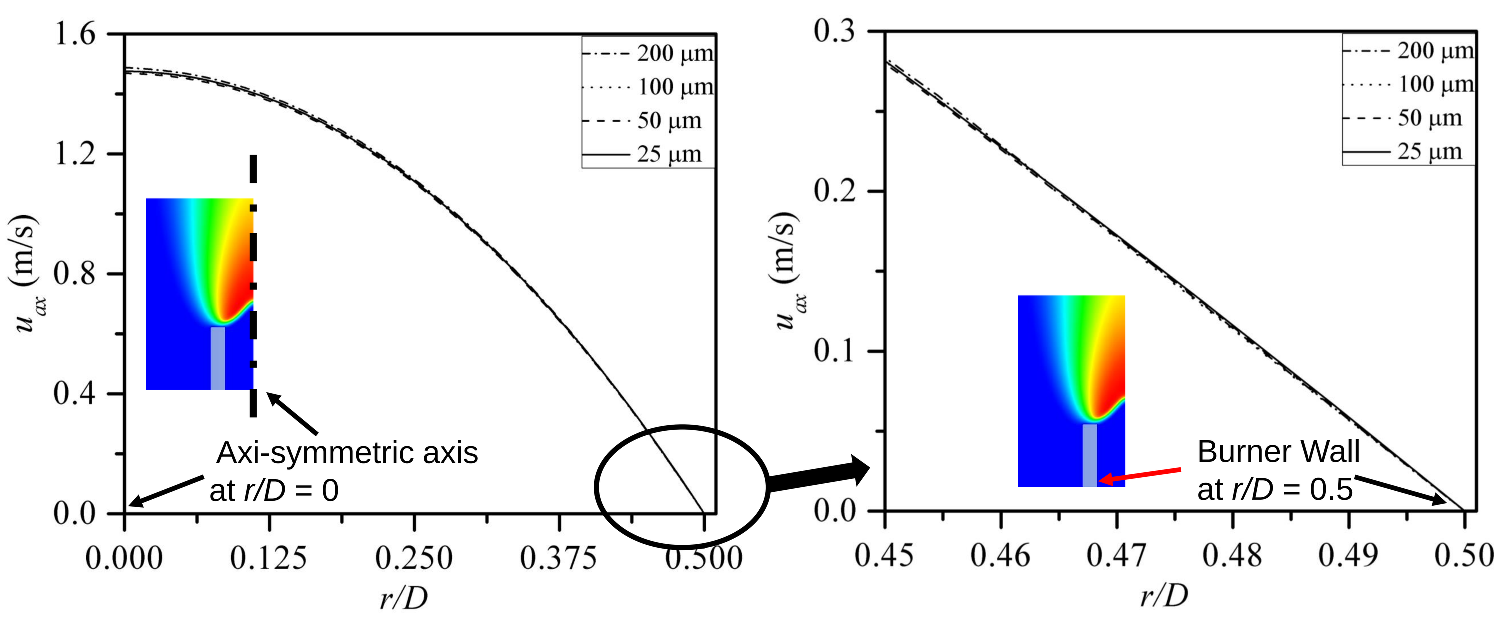


Fig. 7 Variation of axial velocity (u_{ax}) along the radial direction for four grid sizes for lean mixture containing 15 % H_2 (v/v) for D = 2.16 mm at average velocity of 0.7 m/s and axial distance of 49 D

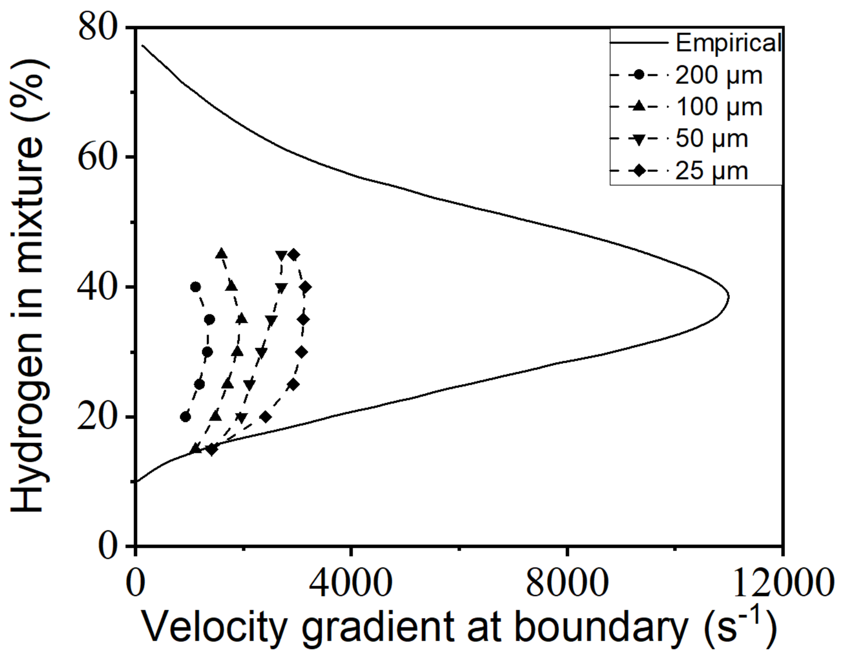


Fig. 6 Comparison of critical velocity gradient ($g = 4V/\pi R^3$) from computations and empirical values obtained value by *Elbe & Morris (1945)*

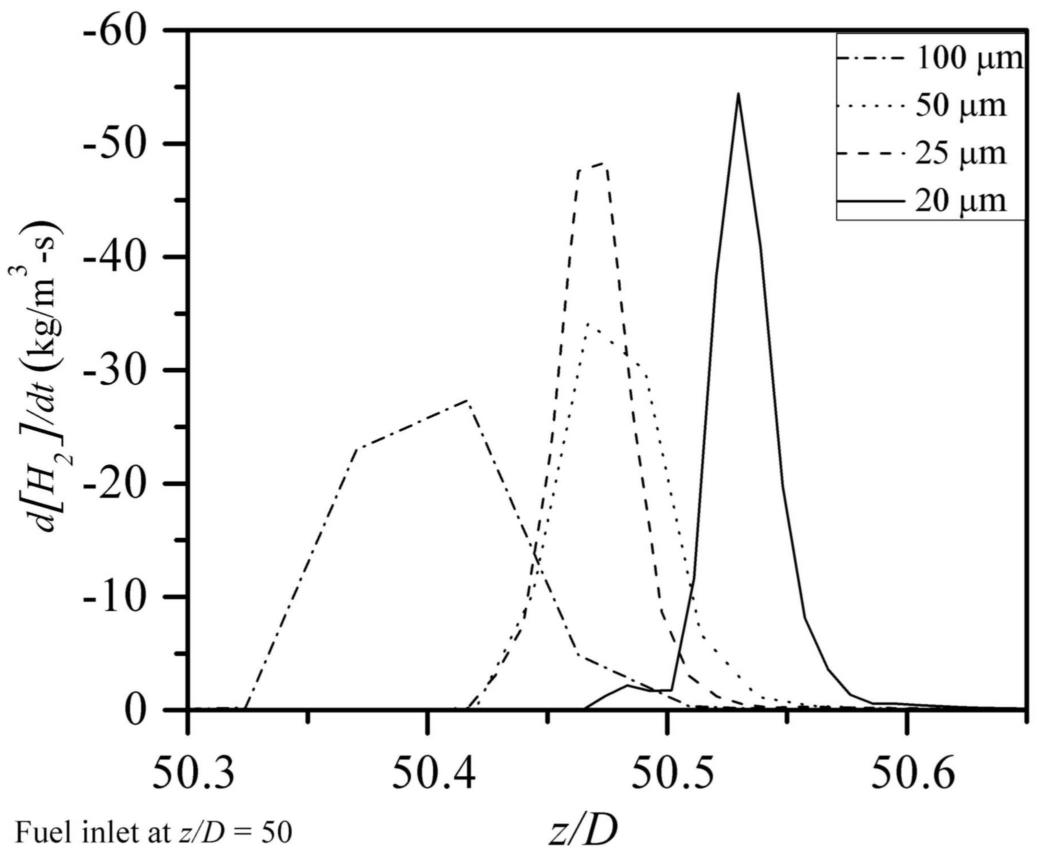


Fig. 8 Variation of net H_2 reaction rate along the axis for four grid sizes for lean mixture containing 15 % H_2 (v/v) for D = 2.16 mm at average velocity of 0.7 m/s

4 Conclusion and future work

- Mesh refinement from 200 to 25 μm shows no change in the axial velocity profile. So, the grid-size which can accurately capture H_2 reaction rate should be used to predict flashback.
- Flame thickness is approximately 100 μm for a lean mixture containing 15 % H_2 (v/v). Hence, course grid sizes (200, 100 and 50 μm) cannot accurately capture the H_2 reaction rate. The H_2 reaction rate profile peak shifts upstream (~0.15mm) with a reduction in grid size (25 to 20 μm). The peak value increases by 12% with a decrease in grid size from 25 to 20 μm for a lean mixture containing 15% H_2 (v/v). Even though the critical velocity gradient (flashback limit) does not show any significant change for the 15% H_2 (v/v) case, the preliminary results cannot recommend a conclusive grid size for convergence for higher H_2% (v/v). Further grid refinement should improve capturing the H_2 reaction rate peak, thus will improve flashback predictions.
- Empirical flashback limit obtained from *Elbe & Mentser (1945)* data also takes into accounts the flashback limit for larger burner diameters (2.16 to 6.6 mm). Hence, the simulations performed with the larger tube diameter will improve the predictions. This is ongoing activity at TU/e as a part of this project.
- Future work involves running transient simulations to further explore the exact cause for flashback for premixed hydrogen flames. Also, these computations will be extended to larger burner diameter transitioning to turbulence. These computational databases will be then used to develop/validated FGM model for predicting flashback [5].

Acknowledgements

- Rijksdienst voor Ondernemend Nederland for financial support for this study (RVO-High Hydrogen Gas Turbine Combustor High Pressure Test DEI120081).
- Power & Flow, Department of Mechanical Engineering, TU/e for providing the computational resources required for the present work

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