Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Advanced Modeling Strategies for Turbulent Hydrogen Flames



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Clusters
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Software
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Institute
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University
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Introduction

The German government's National Hydrogen Strategy has identified hydrogen as a crucial technology in achieving the goals set by the Paris Climate Agreement. Specifically, hydrogen's potential in the transport sector is highlighted, with monovalent hydrogen engines emerging as a promising alternative. However, the combustion of hydrogen presents complex phenomena, driven primarily by its high reactivity and diffusivity. Understanding these phenomena is essential for optimizing hydrogen engine designs, ensuring a safe operation and maximizing their efficiency. Traditional experimental approaches are limited by their complexity and cost, making computational simulations a cost-effective and efficient alternative. Therefore, computational simulations offer a valuable tool for gaining insights into hydrogen combustion processes in a cost-effective and efficient manner. The computational cost of simulating hydrogen combustion is significant, requiring access to high-performance computing (HPC) resources.

Methods

Using OpenFOAM, a computational fluid dynamics (CFD) software, we conducted direct numerical simulations (DNS) to investigate hydrogen combustion. Our focus was on studying the fundamental combustion characteristics of laminar lean hydrogen flames, serving as a foundation for model development. Additionally, we employed the artificially thickened flame (ATF) model and compared it to reference simulations to assess its influence on flame characteristics. The

artifically thickened flame model enables the resolution of the flame front on a coarser grid and therefore leads to a significant reduction of the combutational costs due to less restrictive resolution requirements. OpenFOAM’s capability to accurately solve governing equations, coupled with Python for post-processing, enabled us to investigate phenomena like thermodiffusive instability and cellular structure formation in the flame front.

Results

Simulations of lean hydrogen flames revealed a linear scaling relationship between stability and the thickening factor used in the artificial thickened flame (ATF) model. Under various conditions, stability analyses showed that increasing the thickening factor led to a varying flame stability. These findings offer valuable insights for optimizing the ATF model and improving its predictive accuracy. Additionally, the simulations build the foundation in terms of a quantitative comparison of key characteristics of the fully resolved and partially modeled flames. Moreover, the stability analyses provided insights into the underlying mechanisms governing flame stability, highlighting factors such as flame front curvature and flame speed variations. These insights contribute to a deeper understanding of hydrogen combustion phenomena and enable the refinement of computational models. To advance the modeling in the future towards turbulent hydrogen combustion a stateof- the-art burner was simulated using Large-Eddy Simulation (LES). The burner will be used to evaluate the model performance under controlled and application-oriented conditions. As first step, the flow field of the laboratory burner configuration as well as a pre-cursor LES of an inflow pipe was simulated to obtain qualitative initial and boundary condition of the upcoming reactive simulation.

Discussion

In summary, stability analyses play a crucial role in evaluating computational models and optimizing their predictive capabilities. The insights gained during this project can be directly transferred to model development and extension of the artificial thickened flame model. Finally, a framework for model evaluation under realistic conditions is realized by obtaining initial and boundary conditions of a laboratory burner configuration using LES.

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