

Combustion of Ammonia Blends with Hydrogen/Methane: Simulations with Differential Diffusion and Detailed Chemical Kinetics

アハマド, アーダム

<https://hdl.handle.net/2324/7396276>

出版情報 : Kyushu University, 2025, 博士 (工学), 課程博士
バージョン :
権利関係 :



氏 名 Name : Ahmed Adam

論文名 Title : Combustion of Ammonia Blends with Hydrogen/Methane:
Simulations with Differential Diffusion and Detailed Chemical
Kinetics
(水素およびメタンとアンモニアの混合燃焼：選択拡散と詳細化学反応
を考慮したシミュレーション)

区分 Category : 甲

論文内容の要旨 Thesis Summary

This thesis investigates the influence of differential diffusion on ammonia-based combustion, focusing on its implications for modeling accuracy, flame structure, and pollutant formation. The thesis is divided into five chapters: the first provides an introduction with a literature review, followed by three chapters covering distinct research topics, and finally, Chapter 5 presents the conclusions. Given the rising importance of ammonia and hydrogen as carbon-free fuels, understanding their combustion behavior through high-fidelity simulations is crucial. To this end, both Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES) are employed to study non-premixed flames of NH_3/H_2 and CH_4/NH_3 blends under varying conditions.

In Chapter 2, two-dimensional DNS of NH_3/H_2 non-premixed flames are conducted to evaluate the effect of differential diffusion (DD) by comparing simulations using full multicomponent diffusion with those assuming a Unity Lewis Number (ULN). Flamelet libraries are constructed using both ULN and Constant Lewis Number (CLN) models. The results reveal that the DD case exhibits greater resistance to flame quenching, while the ULN-based models significantly underestimate this stability. The CLN-based flamelet library shows better agreement with the DNS data, indicating the necessity of incorporating differential diffusion effects when modeling hydrogen-containing flames.

Chapter 3 expands the investigation to turbulent NH_3/H_2 flames using DNS in a temporally evolving mixing layer configuration. The study shows that differential diffusion enhances flame stability by promoting increased fuel transport to the flame front and reducing scalar dissipation rates due to smoother species gradients. These effects enable the emergence of partially premixed and premixed flame characteristics even in nominally non-premixed setups. Additionally, the analysis of local diffusion directions reveals a dependence on scalar dissipation rate and flame curvature, providing further insight into ammonia slip and local flame dynamics.

In Chapter 4, the focus shifts to CH_4/NH_3 swirling flames, simulated using LES with the Flamelet-Generated Manifold (FGM) approach. Two diffusion models are assessed: ULN and Mixture-Averaged Diffusion (MAD). While both models predict similar velocity and temperature fields, significant differences arise in species distributions and flame structure due to differential diffusion and Flamelet library interpolation between stable and extinguishing branches. The MAD model leads to broader and overestimated distributions of reactive scalars and NO, while the ULN model aligns more closely with experimental OH and NO profiles. The study also shows that increasing swirl intensity significantly affects flame length and pollutant formation locations, emphasizing the interaction between turbulence and diffusion in determining flame behavior.

Overall, the thesis highlights the inadequacy of simplified diffusion assumptions in ammonia and hydrogen combustion modeling and demonstrates that advanced diffusion models are essential for accurately capturing flame dynamics and emissions. The findings support the development of more reliable Flamelet-based combustion models, which are crucial for the design of next-generation ammonia-fueled combustion systems.