Optimality Comparison of Chemical Kinetic Mechanism for Large Eddy Simulation of Turbulent Non premixed Hydrogen Combustion

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1.Introduction

Hydrogen has appeared as a promising substitute for combustion fuel to facilitate energy transition towards carbon neutrality. However, fuel incompatibility between hydrogen and existing hydrocarbon engines leads to emission and safety issues, resulting in the need to develop a dedicated combustion chamber for hydrogen fuel.

Among existing methods of combustion chamber development, a numerical approach using large eddy simulation (LES) has been established as a design tool for combustion chambers [1]. LES coupled with detailed chemical kinetic mechanism can be used to predict a thermochemical state inside a combustion chamber. Nevertheless, accurate and computationally affordable prediction of temperature and chemical species mass fraction remains difficult to achieve. Therefore, the presented research addresses this issue by presenting optimal comparison between partial and detailed chemical mechanisms in terms of LES predictions and computational cost.

2. Methods

Turbulent non-premixed flame (TNF) case H3 developed by the German Aerospace Center (DLR) was used to validate and assess the prediction accuracy of LES. The specific combustion case H3 was chosen due to strong interaction between turbulence and chemical reactions. Details of parameter regarding case H3 is summarized in Table 1.

Table 1:Specifications of case H3

Parameter	Value/Description
Fuel composition	50% H2: 50% N2 (%v)
Fuel inlet velocity	34.8 m/s
Reynolds number	10,000

Reacting flow solver *reactingFoam* embedded in open-source software, OpenFOAM, was used to solve the governing equations. The chemistry toolkit Cantera was used to modify and load detailed mechanisms. LES computational domain is presented in Figure 1.

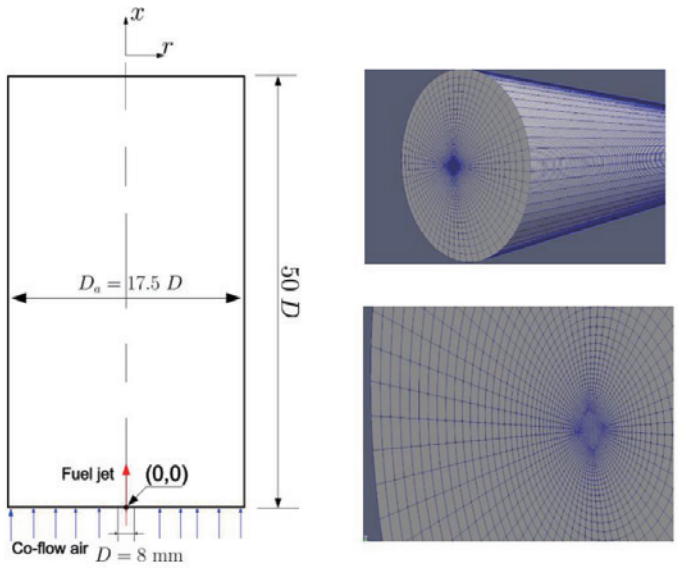

Figure 1: Schematic of computational domain for LES TNF and snapshot of generated mesh.

3. Results and discussion

Grid independence of LES was demonstrated by successive refinement of mesh. Three meshes with increasing cells number (601,600, 1,203,200, and 2,406,400) were employed in LES with a partial Mevel mechanism [2] whose prediction of temperature and reactant species mass fraction are plotted along with the experimental measurement using Raman spectroscopy [3] and Raman-combined with laser-induced fluorescence [4].

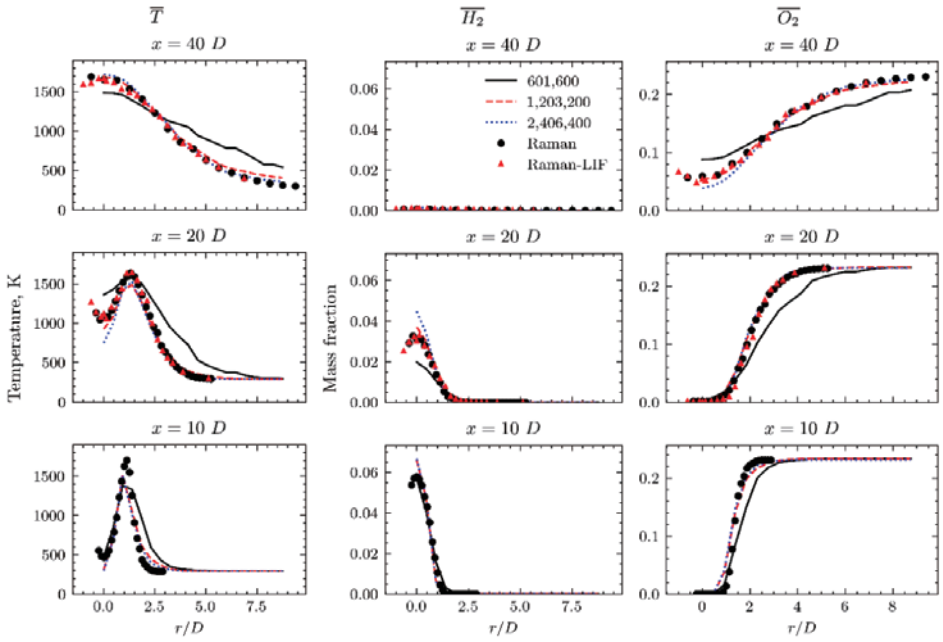

Figure 2: Radial plot of mean simulated and measured temperature and reactant mass fraction using successively refined mesh.

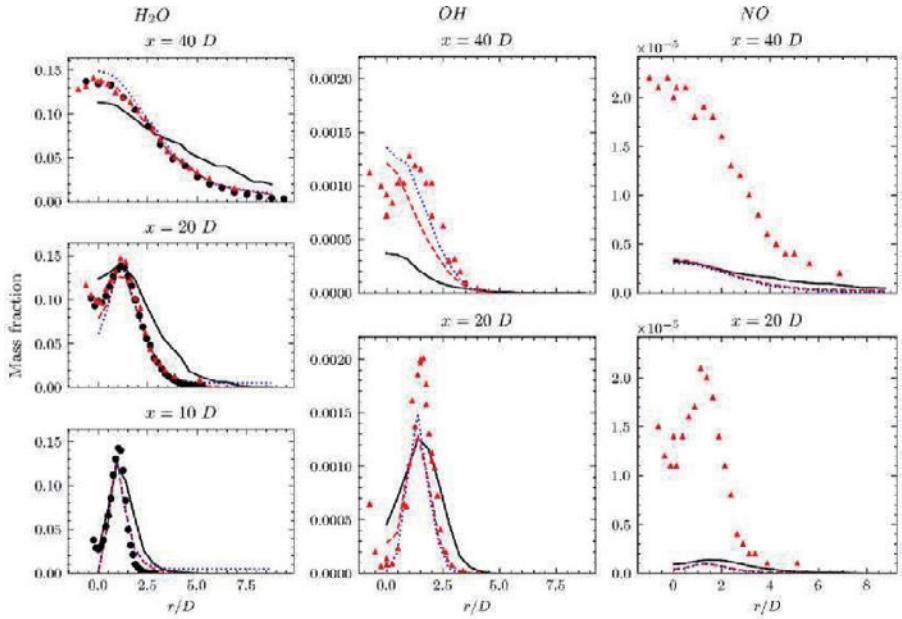

Figure 3: Radial plot of mean simulated and measured product and minor species (OH and NO) mass fraction using successively refined mesh.

Grid independence test shows temperature predicted by LES converges to experimentally measured value with increasing mesh number. The use of intermediate mesh achieves similar prediction accuracy to the more refined mesh, exhibiting grid independence property, and was employed in subsequent LES.

However, increasing mesh cells fail to capture pollutant NO profile. A more elaborate nitrogen chemistry in detailed mechanism is expected to improve NO prediction, albeit with significantly higher computational cost which is subject for future investigation.

4. Summary

LES of TNF based on combustion case DLR-H3 was conducted using a partial chemical mechanism abstracted from detailed mechanism. Grid independence was confirmed at intermediate mesh size around 1.2 milion cells. Further LES using detailed chemical mechanisms is halted due to exponential increases in computational cost.

References

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