The effect of mixture viscosity and thermal conductivity models on a laminar diffusion flame

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Abstract

Laminar hydrogen (H2) diffusion flame is studied using finite-rate chemistry simulation in OpenFOAM. DLBFoam library [1-2] is utilized to speed up chemistry calculations. The simulation results are validated using the experimental data provided by Cheng et al. [3]. Different mixture viscosity and thermal conductivity models are compared, and the effect of viscosity model on the flame structure is described. It is noted that mixing models, utilized in OpenFOAM, might not be suitable for flames with high hydrogen content, let alone pure H2 combustion. Sutherland model utilized for calculating species viscosity and Wilke mixing model results in errors in viscosity prediction of 10-15%. Thus, for combustion problems involving H2, polynomial fitting of species viscosity and thermal conductivity data is recommended in combination with Davidson [4] mixing method. Furthermore, the deviations of the reference data for the viscosity and thermal conductivity for multiple widely used chemical kinetic mechanisms (GRI-3.0, POLIMI, etc.) are also found when compared to experimental data at high temperatures (>1000 K). Open-source CoolProp library [5] exhibits a better agreement with experimental viscosity and thermal conductivity data and therefore is recommended for polynomial fitting.

Keywords: combustion, hydrogen, computational fluid dynamics, OpenFOAM

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