

Ignition Delay Time and Flame Speed Validation of 70-Species Diesel Surrogate Mechanism Using OpenFoam

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Abstract

This case study focuses on the numerical validation of a petrol surrogate using zero-dimensional (0D) ignition delay time (IDT) and one-dimensional (1D) laminar flame speed tests within the open-source CFD software OpenFOAM. Following a comprehensive literature review, the reduced chemical mechanism comprising 70 species and 220 reactions, was selected to accurately represent the surrogate diesel fuel blend containing n-decane, iso-octane, methylcyclohexane (MCH), and toluene. The 0D simulations were conducted using the **chemFoam** solver to determine the IDT at an equivalence ratio of $\phi=0.5$ across pressures of 3 and 7 atm. Subsequently, 1D flame speed simulations were executed using the **reactingFoam** solver within a 1D domain at a set Fuel to air mass Fractions, with the resulting flame speeds post-processed in ParaView. The numerical results were benchmarked and plotted against established experimental data for both IDT[2] and laminar flame speed[3]. This comparison assesses the accuracy of the decoupling methodology mechanism and evaluates the reliability of the OpenFOAM numerical setup for predictive combustion modeling.

Keywords: Diesel surrogate fuel; Skeletal oxidation mechanism; OpenFOAM; chemFoam; reactingFoam;

References

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