FOSSEE, IIT Bombay
OpenFOAM Case Study Project
May 29, 2026

# 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 and laminar flame speed. 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;