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Numerical Investigation of Flame Structure and Soot Formation in Biodiesel Spray Combustion

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We report on Large Eddy Simulations of spray combustion using Karanja Methyl Ester biodiesel, based on the ECN Spray A configuration, which reflects diesel engine conditions with exhaust gas recirculation.
The gas phase is treated numerically in the Eulerian framework, while droplet dynamics are resolved with Lagrangian Particle Tracking. Combustion chemistry is described by a reduced mechanism for a surrogate fuel blend of n-dodecane and methyl butanoate, representative of biodiesel components. This mechanism is tabulated using the Flamelet Generated Manifold (FGM) method, with four control variables: mixture fraction, progress variable, and their variances. Unlike conventional FGM approaches, temperature is not retrieved from the database but is computed directly by solving the energy equation written in terms of sensible enthalpy.
Soot formation is modeled with a detailed phenomenological approach [1], including inception from acetylene (Fig.2), with benzene and pyrene as additional precursors representing PAH chemistry. The model also accounts for surface growth via molecular adsorption, oxidation by O_2 and OH radicals (Fig.3), and particle coagulation. Initially developed for methane flames, it has been adapted for higher hydrocarbons by tuning parameters such as surface growth and oxidation rates to match experimental data.
First, for validation purposes, we present results for n-dodecane and provide comparisons with earlier experimental and numerical data. Subsequently we discuss our simulations of KME spray combustion. More specifically, we present results for important flow properties, including ignition delay time, flame lift-off length, and peak flame temperature, as well as mass fractions of key species and spatial/temporal soot distributions (Fig. 1).

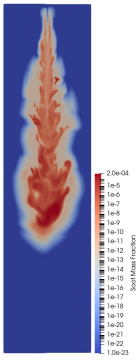

Figure 1: Soot MF

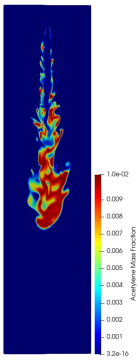

Figure 2: C_2H_2 MF

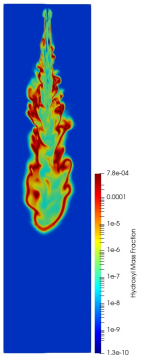

Figure 3: OH MF

References

[1] Zhang M et al. An investigation on early evolution of soot in n-dodecane spray combustion using large eddy simulation. *Fuel*. 2021;293:120072.