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 for Karanja Methyl Ester biodiese. Our numerical setup follows the Engine Combustion Network Spray A configuration, which is representative of of diesel engine operating conditions with exhaust gas recirculation.

The gaseous phase is treated numerically in the Eulerian framework, while the droplet dynamics are resolved via Lagrangian Particle Tracking. A compact chemical kinetics mechanism is employed, featuring a surrogate fuel blend of n-dodecane and methyl butanoate, with the latter representing the ester content of biodiesel[1]). This mechanism is tabulated using the Flamelet Generated Manifold (FGM) methodology. Our FGM formulation incorporating 4 control variables: mixture fraction, progress variable, and their variances (whereas in previous work were only the variance of the mixture fraction was used. This approach ensures accurate yet computationally efficient turbulence-chemistry interaction modeling. Furthermore, the temperature is computed directly by solving the energy equation and is not retrieved from the database, as is typically the case in FGM methodologies.

The soot model (Fig. 1) used in this study follows a multi-step phenomenological approach[2]). It includes soot inception, with acetylene (Fig. 2) being the primary precursor and benzene and pyrene serving as additional precursors, to account for the formation of Polycyclic Aromatic Hydrocarbons. These additional precursors are critical for higher hydrocarbons, as they represent more accurately the complex molecular pathways leading to soot formation under realistic combustion conditions. The model also incorporates surface growth driven by molecular adsorption of these precursors, oxidation mechanisms involving both oxygen and hydroxyl radicals (Fig. 3), and coagulation of soot particles to account for changes in particle size and number density. Initially developed and calibrated for methane flames, this model has been extended to capture soot dynamics in diesel and biodiesel sprays by tuning key constants, such as those governing surface growth and oxidation rates, to match experimental data.

We present results for key global flame properties, including ignition delay time, flame lift-off length, and peak flame temperature. We examine the mass fractions of species linked to combustion efficiency and soot formation, along with spatial and temporal soot concentration profiles. Finally, the numerical findings are compared against experimental and computational data for diesel and its surrogate, n-dodecane.

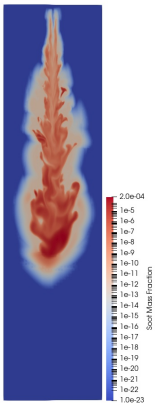

Figure 1: Soot Mass Fraction

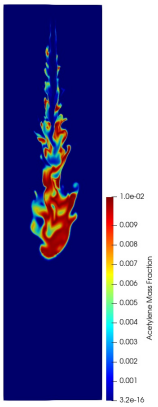

Figure 2: C_2H_2 Mass Fraction

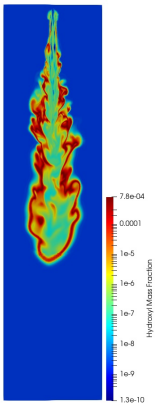

Figure 3: OH Mass Fraction

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[1] Sula et al., *Combustion and Flame* **Volume 249**, 112611 (2023)

[2] Zhang et al., *Fuel* **Volume 293**, 120072 (2021)