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Development of a Multi-Component Surrogate Model for Biodiesel Fuel

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The global shift toward carbon neutrality is accelerating the use of alternative diesel fuels such as fatty acid methyl esters (FAME) and hydrotreated vegetable oil (HVO). Because variations in fuel composition significantly affect combustion and emissions, robust engine-design methodologies that can accommodate multiple fuel types are required. Although three-dimensional CFD coupled with detailed chemical kinetics is a powerful tool, conventional surrogate fuel models rely on only a few gas-phase species and cannot reproduce liquid-phase properties such as distillation behavior.

This study proposes a multi-component surrogate strategy that decouples liquid-phase and gas-phase surrogates to simultaneously capture physical and chemical characteristics of biodiesel-blended diesel fuels. Four fuels were investigated: B7 (7% bio-blend diesel), HVO, PME50 (50% palm methyl ester blend), and SME50 (50% soybean methyl ester blend). Engine experiments were conducted using a four-cylinder diesel engine under four operating conditions, while soot distributions were measured in an optically accessible Rapid Compression and Expansion Machine (RCEM) using two-color pyrometry, where KL (line-of-sight soot optical thickness) was derived from luminous-flame images. CFD spray combustion simulations were performed with the SAGE detailed chemistry solver.

Liquid-phase surrogates consisting of 36 components were constructed directly from fuel composition data by assigning representative species for each hydrocarbon class and carbon number; this approach reproduces distillation curves through Raoult's law without empirical fitting and allows consistent surrogate construction for new fuels from analysis data. Gas-phase surrogates comprising 13 representative species were mapped to a detailed kinetic mechanism based on CRECK (combustion kinetics framework). To match fuel reactivity, cetane number (CN) equivalence was achieved through a four-step calibration, followed by a global multiplier for final ignition phasing. The base detailed mechanism was reduced and augmented with sub-mechanisms relevant to soot precursors and emissions, yielding a reduced mechanism of 284 species and 5,842 reactions that is practical for 3D-CFD in practice.

Figure 1 shows that simulated distillation curves closely follow experimental measurements for all four fuels, confirming that the 36-component liquid surrogate robustly captures fuel-specific vaporization behavior across paraffinic and ester-containing blends. Engine validation demonstrates that cylinder pressure traces, heat-release histories, and ignition-delay trends are reproduced with good agreement across fuels and operating conditions.

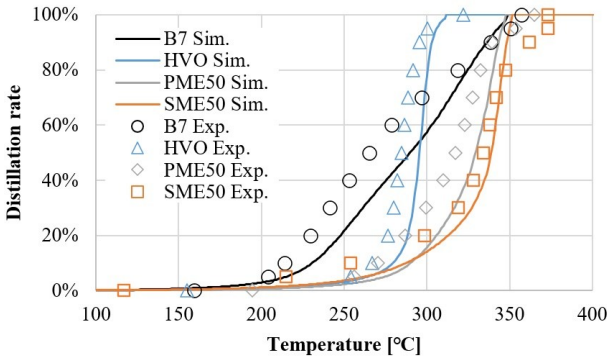

Figure 1. Comparison of simulated and experimental distillation curves

Figure 2 compares CFD-predicted soot number density distributions with experimentally visualized KL in the RCEM under Condition 2 (1600 rpm, 20 mm³/st, EGR 34%), and the simulations qualitatively reproduce fuel-dependent soot evolution and spatial distribution: HVO shows soot formation concentrated near the spray center at early stages, whereas B7 exhibits stronger soot formation near the bowl lip during the soot peak period.

Emission trends for NOx and total hydrocarbons (THC) are captured well overall, while soot is overpredicted for SME50, suggesting that soot oxidation behavior in FAME-rich fuels remains sensitive and that further refinement of FAME-specific pathways and PAH (polycyclic aromatic hydrocarbons) / soot sub-mechanisms is required. Overall, the proposed decoupled surrogate framework, requiring only fuel composition data and standard fuel properties, provides a systematic, transferable, and composition-driven methodology for virtual screening and comparative assessment of emerging biofuels and synthetic fuels during early-stage engine development, reducing the need for extensive hardware testing for each new fuel formulation.

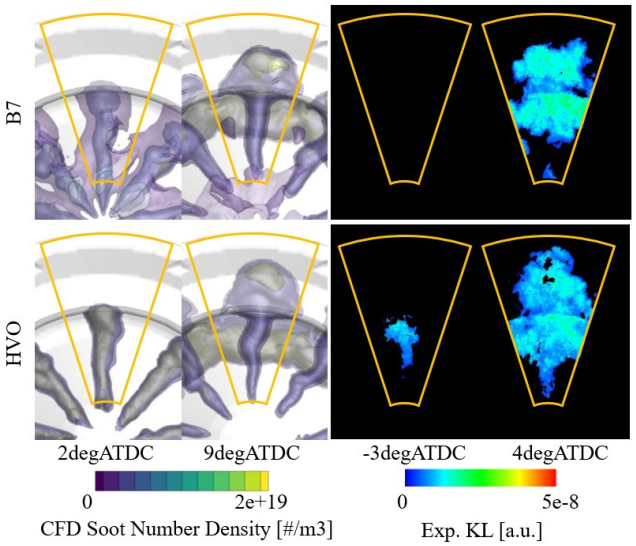

Figure 2. Comparison of CFD soot number density iso-surfaces and visualized KL under Condition 2 (1600 rpm, 20mm³/st, EGR 34%) (top: B7, bottom: HVO; left: early soot formation, right: soot peak period; orange line: KL visualization area).