Kinetic Modelling, Life Cycle Assessments, and Cetane Number Analysis of Alcohol-to-Jet Fuel to Reduce CO2 Emissions

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The aviation sector contributes approximately 2.5% of global CO2 emissions, emphasizing the urgent need for sustainable alternatives to conventional jet fuels. This study aims to evaluate the combustion characteristics of alcohol-to-jet (ATJ) fuels to determine their potential for reducing emissions and ensuring compatibility with current aviation engines. Ignition delay times (IDTs) were measured in a constant-volume combustion spray chamber under low-temperature oxidation and engine-relevant conditions. Chemkin-Pro simulations were used to model combustion kinetics. Experimental IDTs closely matched those simulated for 2,2,4-trimethylpentane (iC8), 2,2,4,4,6,8,8-heptamethylnonane (iC16), and their mixtures, validating the kinetic models and confirming the accuracy of the functional group-based surrogate formulation. To meet cetane number (CN) requirements, dodecane was blended at 35–60% levels, significantly enhancing ignition quality. IDT measurements showed typical reactivity trends with temperature and pressure, supporting ATJ fuel's suitability for current engine operations. Derived CNs of batches 2, 3, and 4 complied with ASTM certification standards and demonstrated reduced susceptibility to lean blowout. Key combustion pathways were identified as hydrogen abstraction reactions, and an AI model accurately predicted CN based on blend composition. A well-to-wake life cycle assessment (LCA) conducted in Saudi Arabia showed a 27.03% reduction in CO2 emissions compared to conventional jet fuel, underscoring ATJ's promise as a sustainable aviation fuel.

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