

## Development of a Reduced Biodiesel Surrogate Fuel Model for Multi-Dimensional CFD Simulations

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**Abstract:** This work reports the development of a reduced biodiesel surrogate fuel model for multi-dimensional CFD simulations. The model is derived using an integrated kinetic mechanism reduction scheme and the final chemistry comprises only 83 species. The model is first validated in zero-dimensional (0-D) chemical kinetic calculations under a wide range of auto-ignition and jet-stirred reactor (JSR) conditions. The computed ignition delays (ID) and species profiles are in well agreement with those of the detailed model. Besides, the experimental species profiles of rapeseed methyl ester (RME) oxidation in a JSR are also reasonably reproduced. Subsequently, the fidelity of the model is further assessed in two-dimensional (2-D) CFD simulations of a constant-volume combustion vessel with respect to the experimental results of soy-methyl ester (SME) combustion. Comparisons of the computations with the experimental data reveal that ID, lift-off lengths (LOL) and soot volume fractions are reasonably well replicated by the model. Successively, the applicability of the reduced model to serve as a universal surrogate model for other biodiesel feed-stocks, such as palm-methyl ester (PME) and sunflower-methyl ester (SFME), is investigated in both 0-D and 2-D simulations. The compositions of the reduced model are varied according to the saturation/unsaturation levels in each fuel. In this work, it is demonstrated that the reduced model can potentially be used to predict the reactivity of biodiesel feed-stocks with low degree of saturation ( $\leq 30\%$ ) in both kinetic and CFD spray simulations.

**Keywords:** Chemical kinetics; Mechanism reduction; Biodiesel; CFD; Spray combustion