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On Formulating a Simplified Soot Model for Diesel and Biodiesel Combustion

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In this study, a semi-empirical two-equation soot model that can predict soot in petrodiesel and biodiesel sprays and quantitative differences between soot volume fractions in the two sprays under engine conditions is developed. n-Heptane is used as the surrogate for petrodiesel and a ternary mixture of methyl decanoate, methyl-9-decanoate, and n-heptane as the surrogate for biodiesel. The n-heptane simulations are conducted using a 160-species mechanism. In the case of the ternary biodiesel surrogate, a 115-species reduced mechanism is employed to model the chemical kinetics. The semi-empirical soot model includes soot inception, surface growth, coagulation, and also oxidation. The results from the semi-empirical model will be compared to those obtained from a detailed soot kinetics model in one-dimensional diffusion flame studies. Analysis of the results shows that the model developed in this work can predict soot formation at various conditions for both petrodiesel and biodiesel fuels reasonably well, and at a fraction of the computational cost of the detailed soot kinetics mechanism.

Keywords: Biodiesel combustion; Soot formation; Reaction pathway analysis; Flamelets; Two-equation soot model; Reacting sprays.

1. Introduction

In conventional compression-ignition engines, fuel is injected directly into the cylinder toward the end of the compression stroke and it auto-ignites. Combustion primarily occurs in highly strained and wrinkled diffusion flames surrounding the fuel jet and located where the fuel/air mixture is stoichiometric. Polycyclic aromatic hydrocarbons (PAHs) are formed in the rich mixture downstream of the flame lift-off height and eventually form soot farther downstream [1,2]. Soot is a harmful by-product of combustion that is known to be harmful to human health and the environment [3-7]. As such, soot emissions from engines are strictly regulated. Predictive models for soot can aid engine designers in their efforts to develop cleaner engines. However, the modelling of soot is challenging because the kinetic mechanisms of soot formation, the turbulence/chemistry interactions

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