

Effects of fuel preheat temperature on soot formation in methyl linolenate co-flow diffusion flames

Royston Mwikathi Kiraithe  and Josephat Kipyegon Tanui

Department of Mechanical Engineering, Dedan Kimathi University of Technology Private Bag 10143, Nyeri, Kenya

ABSTRACT

The objective of this study was to investigate the mechanism of soot formation in biodiesel by analyzing the combustion of individual components. The paper presents a numerical analysis of the effect of preheat temperatures on nucleation rates, coagulation rates, and soot volume fraction in methyl linolenate (MLE) co-flow flame. In this work, Moss-Brooke's soot model and a reduced kinetic mechanism containing 177 chemical species and 2904 chemical reactions were used to simulate the pyrolysis and combustion of MLE. A laminar jet flame with inlet velocities of 0.4 m/s was studied. The preheat temperature of the fuel was varied between 300 and 450 K. The burner walls were stationary and no-slip conditions were applied. The pressure outlet had Neumann boundary conditions and the tangential velocity was set to zero at the wall. It was established that an increase in fuel preheat temperatures causes an increase in nucleation rates and the amount of soot due to accelerated fuel pyrolysis, improved diffusion, acceleration from buoyancy, and earlier formation of PAHs. It was discovered that increasing the fuel preheat temperature had a greater impact on soot formation along the centerline than on the wing.

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1. Introduction

High population growth and environmental degradation are some of the key factors that demand a search for a substitute fuel (Mao et al., 2020). Biodiesel is one of the fuels that can be used as an alternative because it is environmentally friendly and can be synthesized from renewable materials. Biodiesel consists of five major components. The constituents are methyl linolenate (MLE), methyl linoleate (MLi), methyl oleate (MO), methyl palmitate (MP), and methyl stearate (MS), the proportions of these methyl esters vary depending on the type of feedstock (Hoekman et al., 2012).

Soot contributes significantly to particulate emission from hydrocarbon combustion (Johnson and Joshi, 2018). Soot in flame is caused by incomplete combustion of hydrocarbons due to insufficient oxygen required to convert fuel to carbon dioxide and water vapor (Vinayagam et al., 2021). To reduce soot emissions, the effect of controlling parameters on soot formation has been extensively researched (Mazzei et al., 2017), e.g.,

composition of fuel (Gu et al., 2016), temperature (Sun et al., 2017) and pressure (Sarnacki and Chelliah, 2018).

A complex chemical process (gas-phase process) and a physical process combine to form soot (soot particle dynamics). The formation of soot begins with pyrolysis and oxidation, followed by combination and cyclization reactions that result in the formation of polycyclic aromatic hydrocarbons (PAHs) (Frenklach and Wang, 1994). Polycyclic aromatic hydrocarbons nucleate as they grow, resulting in the formation of soot. Following nucleation, the primary soot particles congeal and develop a surface (Mazzei et al., 2017). Surface growth is caused by the condensation of polycyclic aromatic hydrocarbons and hydrogen abstraction carbon addition (HACA) surface growth mechanism. This expansion is responsible for an increase in the size and mass of soot particles (Celnik et al., 2009). Primary particles collide to form particle aggregates that resemble chains. Because the soot is formed at high temperatures, it is constantly accompanied by oxidation. O₂ and OH both play important roles in oxidation (Westbrook et al., 2009).

CONTACT Royston Mwikathi Kiraithe  kiraitheroyal@gmail.com  Department of Mechanical Engineering, Dedan Kimathi University of Technology Private Bag 10143, Nyeri, Kenya

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