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Discrete multicomponent model for biodiesel spray combustion simulation

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HIGHLIGHTS

- Discrete and continuous multicomponent liquid models are calculated from the real biodiesel properties.
- Continuous multicomponent liquid model is employed for diesel spray simulation.
- The predicted spray-combustion characteristics of diesel and biodiesel are compared with the experimental measurements.
- The discrete model performs better than the continuous model in predicting the spray-combustion characteristics of the biodiesel flame.
- Effects of the relative abundance and the relative volatility of biodiesel fuel components are highlighted.

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ABSTRACT

An important first step in spray combustion simulation is an accurate determination of the fuel properties which affects the modelling of spray formation and reaction. In a practical combustion simulation, the implementation of a multicomponent model is important in capturing the relative volatility of different fuel components. A Discrete Multicomponent (DM) model is deemed to be an appropriate candidate to model a composite fuel like biodiesel which consists of four components of fatty acid methyl esters (FAME). In this paper, the DM model is compared with the traditional Continuous Thermodynamics (CTM) model for both diesel and biodiesel. The CTM model is formulated based on mixing rules that incorporate the physical and thermophysical properties of pure components into a single continuous surrogate for the composite fuel. The models are implemented within the open-source CFD code OpenFOAM, and a semi-quantitative comparison is made between the predicted spray-combustion characteristics and optical measurements of a swirl-stabilised flame of diesel and biodiesel. The DM model performs better than the CTM model in predicting a higher magnitude of heat release rate in the top flame brush region of the biodiesel flame compared to that of the diesel flame. Using both the DM and CTM models, the simulation successfully reproduces the droplet size, volume flux, and droplet density profiles of diesel and biodiesel. The DM model predicts a longer spray penetration length for biodiesel compared to that of diesel, as seen in the experimental data. Also, the DM model reproduces a segregated biodiesel fuel vapour field and spray in which the most abundant FAME component has the longest vapour penetration. In the biodiesel flame, the relative abundance of each fuel component is found to dominate over the relative volatility in terms of the vapour species distribution and vice versa in the liquid species distribution.

1. Introduction

Growing interest in biodiesel as a renewable fuel has triggered many studies to understand the spray-combustion characteristics of the new fuel. Application of biodiesel in unmodified engines requires similar combustion characteristics to those of conventional fuel. Experiments have suggested that differences in fuel physical and chemical properties lead to different spray characteristics such as droplet size [1–3], spray penetration [4], and spray cone angle [5]. Changes in combustion behaviour in terms of emissions [1–3,6], burning velocity [1,7], flame temperature [9], and flame height [6] are observed by switching from conventional fuel to biodiesel. Simulating the differences in spray-combustion characteristics of different fuels is a challenge that requires an

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Nomenclature

air	air parameter
-	averaged quantity
atom	atomising air parameter
z	axial location
z	axial parameter
b	biodiesel parameter, boiling parameter
ch	characteristic parameter
I	chemiluminescence intensity
d	diameter
d	diesel parameter,droplet parameter
ρ	density
N	droplet number
ϕ	equivalence ratio
*i*th	fuel component properties
$\dot{q}$	heat release rate per unit volume
q	heat release rate
i	*i*th computational parcel properties
inject	injection parameter
m	mass
$\dot{m}$	mass flow rate
Y	mass fraction
max	maximum variable
r	radius
r	radial parameter
δ	Rosin–Rammler characteristic droplet diameter
swirl	swirl air parameter
D_{32}	Sauter mean diameter
T	temperature
D_{30}	volume mean diameter
V	volume flux
U	velocity
^	normalised parameter

acronym

CFD	Computational Fluid Dynamics
CTM	Continuous Thermodynamics Model
CTRZ	central top reaction zone
DM	discrete multicomponent model
FAME	fatty acid methyl esters
GC	Gas Chromatography
IDEA	Integrated Diesel European Action
IDEA-CTM	IDEA with Continuous Thermodynamics Model
OpenFOAM	Open Source Field Operation and Manipulation
PSR	Perfectly Stirred Reactor
PaSR	Partially Stirred Reactor
PDA	Phase Doppler Anemometry
PISO	Pressure Implicit Split Operator
PIV	Particle Image Velocimetry
PME	Palm Methyl Ester
PME-CTM	Palm Methyl Ester with Continuous Thermodynamics Model
PME-DM	Palm Methyl Ester with Discrete Model
TAB	Taylor Analogy Breakup
URANS	Unsteady Reynolds Average Navier Stokes

evaluation of the sensitivity of available (CFD) tools towards fuel properties, and this point is discussed in the present study.

Much work has been done on the effects of the fuel chemical properties in spray combustion modelling [11,12,20] but there are relatively few studies on the effects of the fuel physical properties [14,17]. Before employing a complex and expensive chemistry calculation, the effects of the fuel physical properties need to be understood. The present study decouples the effects of chemistry by comparing models for the liquid fuel properties using an identical chemical mechanism for all fuels considered. Therefore, the effects of the liquid physical properties on spray-combustion characteristics can be studied systematically in isolation.

Different experimental [10,15] and numerical studies [16,34-36] have concentrated on the importance of evaporation in the spray combustion process. Modelling the spray formation and evaporation of practical fuels requires the implementation of a multicomponent model to capture the relative volatility effects. Two approaches have been used in the implementation of multicomponent models, known as the Discrete Multicomponent (DM) model [34,36] and the Continuous Thermodynamics (CTM) model [12,20,35]. The DM model represents each pure component discretely while the CTM model combines all the pure components properties into a single continuous surrogate. Most fossil fuels are modelled with the CTM approach due to its modelling simplicity. Hundreds of components are simplified by a few representative surrogates in the calculation of the pure component properties before the application of mixing rules to formulate a single continuous set of physical properties.

In the case of a composite fuel like biodiesel that consists of only four main fatty acid methyl ester (FAME) components [25], DM is a practical modelling approach. However, many biodiesel computational studies have been done based on the traditional CTM approach [12,20,35] due to the simplicity of the modelling, which may not be appropriate for biodiesel. A DM approach has been applied to bio-oil evaporating spray [35] and a similar approach has been applied to model decane-heptane evaporating spray [36]. Both of these studies were based on a non-reacting spray, but the present study is intended to observe the effect of combustion on the multicomponent spray formation process. The importance of the relative volatility of different components in the predicted fuel vapour fields has been considered previously [35]. The present study extends the discussion based on a reacting case to illustrate the competition between the relative volatility and the relative abundance of the fuel components in the predicted spray and combustion behaviour.

Prediction methods for FAME pure components have been developed and validated recently, aimed at further studies of biodiesel using the DM method [37]. The CTM method [12,20] involves some compromise on the accuracy of the volatility properties due to the implementation of mixing rules on a composite fuel like biodiesel. A well-established (GC) dataset [25] on biodiesels derived from palm oil, Palm Methyl Esters (PME), is incorporated in the DM model.

Validation of spray combustion simulations has been a limitation on their usefulness [31] due to the complex interplay between different physical processes. Therefore, validation studies of unsteady spray combustion simulations have been limited to macro-scale characteristics such as spray penetration, spray shape, flame shape and global droplet size [19,20]. Validation of the micro-scale characteristics such as local droplet size, droplet flux, and velocity profiles have been limited to sprays of a single component fuel [24]. Hence, the present study aims to validate the same micro-scale spray characteristics for practical fuels. Since there is no validation effort for the multicomponent model that extends to reacting sprays, the present study provides a semi-quantitative validation of the spray and combustion characteristics that