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Vaporization modeling of petroleum–biofuel drops using a hybrid multi-component approach

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ABSTRACT

Numerical modeling of the vaporization characteristics of multi-component fuel mixtures is performed in this study. The fuel mixtures studied include those of binary components, biodiesel, diesel–biodiesel, and gasoline–ethanol. The use of biofuels has become increasingly important for reasons of environmental sustainability. Biofuels are often blended with petroleum fuels, and the detailed understanding of the vaporization process is essential to designing a clean and efficient combustion system. In this study, a hybrid vaporization model is developed that uses continuous thermodynamics to describe petroleum fuels and discrete components to represent biofuels. The model is validated using the experimental data of n-heptane, n-heptane–n-decane mixture, and biodiesel. Since biodiesel properties are not universal due to the variation in feedstock, methods for predicting biodiesel properties based on the five dominant fatty acid components are introduced. Good levels of agreement in the predicted and measured drop size histories are obtained. Furthermore, in modeling the diesel–biodiesel drop, results show that the drop lifetime increases with the biodiesel concentration in the blend. During vaporization, only the lighter components of diesel fuel vaporize at the beginning. Biodiesel components do not vaporize until some time during the vaporization process. On the other hand, results of gasoline–ethanol drops indicate that both fuels start to vaporize once the process begins. At the beginning, the lighter components of gasoline have a slightly higher vaporization rate than ethanol. After a certain time, ethanol vaporizes faster than the remaining gasoline components. At the end, the drop reduces to a regular gasoline drop with heavier components. Overall, the drop lifetime increases as the concentration of ethanol increases in the drop due to the higher latent heat.

1. Introduction

Due to the importance of drop vaporization to liquid fuel combustion, a large number of experimental and numerical studies have been conducted on this topic [1–3]. This paper focuses on drop vaporization modeling, which is a classical research area related to fuel combustion. There are numerous aspects associated with vaporization modeling, including hydrodynamics, heat transfer, and the effect of fuel components. The present study emphasizes on the modeling of the effect of fuel components.

For numerical modeling, in addition to the traditional method of using the single-component approach, various methods of using the multi-component approach have been proposed. Multi-component approaches can be classified into two major categories: discrete component and continuous thermodynamics. The discrete component approach is characterized by the premise that the complex multi-component fuel is a mixture of several representative species. One such typical approach uses six species for diesel fuel and seven species for gasoline for vaporization modeling [4]. Similar approaches were also used to model liquid fuel vaporization based on the discrete component approach [5–7]. On the other hand, continuous thermodynamics uses a continuous distribution function to model the composition of a complex fuel. A gamma distribution was first developed and used to represent the molecular weight distribution of petroleum fuels for vaporization modeling [8]. The same approach was adopted and further improved by others to model spray vaporization in practical combustion environments [9–11]. Similar methods based on continuous thermodynamics were also developed and applied to simulate jet fuel vaporization [12] as well as other applications [13]. In addition to the above two main categories, other methods, such as those based on the kinetic theory and the distillation curve, were also proposed. A detailed review of drop vaporization modeling was reported by Sazhin [3].

Since the mixtures of different fuels are frequently used in industry, research on the vaporization of the mixture of two or more fuels with different properties has been emphasized. Sirignano et al. [2,14] introduced the concept of mass flux potential and derived a detailed approach to model the vaporization of

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multi-component fuel drops in a cubic drop array. The single-component model by Abramzon and Sirignano [15] was extended to simulate the vaporization of binary-component drops (n-heptane–n-decane) at different fuel ratios, and good levels of agreement between simulations and experiments were obtained [16]. Stengele et al. [17] numerically studied the vaporization of n-pentane–n-nonane mixture in a high pressure convective flow and also conducted experiments to verify the numerical results. The above vaporization models for fuel mixtures are mainly for drops blended by multiple single-component fuels (e.g., n-heptane and n-decane). On the other hand, blends of practical multi-component fuels with distinct properties, such as the mixture of biofuel and petroleum fuel, are frequently used in combustion devices such as internal combustion engines. Therefore, research on the vaporization of fuel drops that are mixtures of different practical fuels is needed. In modeling the vaporization of practical fuel blends, the variation in the composition, resulting from the differences in vaporization rates and liquid phase diffusion in the fuel mixture, needs to be considered.

The questionable future availability of petroleum fuels and the concern about environmental carbon emissions require more research and application of renewable fuels. Biofuels, as the promising renewable substitution for petroleum fuels, are being used in many combustion devices. With comparable physical and chemical properties, for instance, biodiesel can be used as the partial replacement for diesel fuel, and ethanol can be used together with gasoline. Experimental studies showed that comparable engine performance and improved emissions of carbon monoxide, unburned hydrocarbon, and soot can be obtained by using biodiesel, with a slight penalty in nitrogen oxides emissions [18–21]. A practical way of utilizing biodiesel is to blend it with diesel fuel due to their high miscibility. In this case, significant modifications to the engine are not required. Research has been conducted on engine performance using the blend of diesel fuel and various kinds of biodiesel with different blend ratios. It was found that the volume fraction of biodiesel can be up to 20%, around which an optimum engine thermal efficiency can be obtained without a significant increase in nitrogen oxides emissions [18,20,22,23]. Despite the extensive engine studies, there are only limited studies on the vaporization of the mixture of biofuels and petroleum fuels at a fundamental level.

One challenge in modeling biodiesel vaporization is the uncertainty of the fuel property. Vegetable oils, such as rapeseed methyl ester, soybean methyl ester, and sunflower methyl ester, are commonly used to produce biodiesel. Different feedstock leads to different compositions. Therefore, the physical properties of biodiesel can be relatively uncertain. However, despite the difference in feedstock, most biodiesel derived from vegetable oils is mainly composed of five C16–C18 fatty acids [20,24], namely, palmitic ($C_{16}H_{32}O_2$), stearic ($C_{18}H_{36}O_2$), oleic ($C_{18}H_{34}O_2$), linoleic ($C_{18}H_{32}O_2$), and linolenic ($C_{18}H_{30}O_2$). Ramos et al. [24] studied the effect of the raw material composition on biodiesel properties. Wu et al. [25] tested the effect of feedstock of biodiesel on diesel engine emissions using five different methyl esters. Yuan et al. [26,27] also provided methods to predict the physical properties of biodiesel using the above five fatty acids with an ideal mixing rule. Based on the mixing rule, the physical properties of biodiesel can be predicted according to the mass fractions of these components.

To help understand the biodiesel combustion process, a better understanding of biodiesel drop vaporization characteristics is required. The vaporization of biodiesel drops was studied experimentally and numerically only recently. Morin et al. [28,29] measured the drop size histories during the vaporization of rapeseed methyl ester and sunflower methyl ester. Barata [30] numerically simulated the dispersion and vaporization of rapeseed methyl ester drops that were injected into a turbulent cross-stream and compared the results with those using conventional fuels. Traditionally the modeling of diesel–biodiesel vaporization has been based on well-defined properties of the two fuels and thus is essentially a binary-component approach [31,32]. In this approach, both diesel fuel and biodiesel are treated as two single-component fuels. Despite the increasing importance of biodiesel–petroleum fuel blends, a vaporization model that considers the complex fuel components is not currently available.

The purpose of this paper is to model the vaporization of the mixtures of petroleum fuels and biofuels under high temperature conditions. A vaporization model and a method of predicting the physical properties of biodiesel are presented. The model is first validated by predicting the vaporization of single-component and binary-component drops. The model is applied to simulate the vaporization of biodiesel, diesel–biodiesel, and gasoline–ethanol drops. The present research is essential for the further modeling of spray combustion in engines using biofuels.

2. Model formulation

The model developed in this paper is capable of predicting the vaporization of single-component drops (e.g., n-heptane) and multi-component drops. The multi-component drops include those of binary-component mixtures (e.g., n-heptane and n-decane), petroleum fuels (e.g., diesel and gasoline), biofuels (e.g., biodiesel), and blends of petroleum and biofuels (e.g., diesel–biodiesel and gasoline–ethanol). The vaporization of multi-component drops differs from that of single-component drops not only because the physical properties are different, but also the composition of the drop changes during the vaporization process. The above multi-component fuels vary significantly in the nature of their compositions and thus require different modeling approaches. For the n-heptane–n-decane mixture, the drop is modeled using a blend of two single components with well-defined properties. The petroleum drop is composed of hundreds of hydrocarbon species and is modeled using a continuous thermodynamics approach to represent the molecular weight distribution. Biodiesel also consists of many oxygenated hydrocarbon species but mostly contains five major species; thus, biodiesel is simulated using five discrete components. On the other hand, the diesel–biodiesel drop is described by a combination of continuous distribution and discrete components, as is the gasoline–ethanol drop. As a result, the present model can be regarded as a hybrid model.

This section first describes the formulation of the multi-component vaporization model that is applicable to all the drops studied in this paper. Next, the formulation to describe the petroleum fuel composition is discussed. Additionally, for multi-component drops, the vaporization modeling also relies on the accurate prediction of the physical properties of the fuels. Thus, a method to evaluate biodiesel properties is also described.

For clarification, in this paper the word "fuel" is used to represent a fuel in its original form. Therefore, it can mean n-heptane, biodiesel, or diesel. The latter two are multi-component in nature. Additionally, different components in the same fuel are assumed to have the same vapor diffusivity. The liquid drop is assumed to have a uniform composition, as is discussed later. The above assumptions are employed in order to reduce the complexity of modeling the diffusion of hundreds of species in a practical fuel (e.g., diesel) and are also due to the data availability.

2.1. Drop vaporization model

The vaporization of a multi-component liquid fuel mixture involves the transport of the various fuel vapor components in the gas phase surrounding the drop. It is assumed that the drop