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Effect of droplet sizes on evaporation of a bi-component droplet at DME (dimethyl ether)/n-heptane-fueled engine conditions

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ABSTRACT

Two fuels with the compression-ignition property similar to conventional diesel—DME and n-heptane—are selected to analyze the evaporation performance of a bi-component droplet at different internal combustion engine conditions. A multi-component evaporation model based on UNIFAC (Universal Functional Activity Coefficient) method and the non-equilibrium evaporation law is implemented to predict the evaporation characteristics of "each component" of the DME/n-heptane droplets with different mass fractions and different initial diameters, and to find how the two main competing factors (the consumption of latent heat for evaporation and the heat transfer into the droplet) affect the evaporation behaviors of each component. Generally, reducing the mass fractions of DME, increasing the ambient temperature or increasing the relative velocity between the droplet and the ambient gas enhances the evaporation of a droplet. Decreasing initial droplet diameter reduces the "peak" evaporation rate of both components. It is interesting to find that a relative constant and high evaporation rate of DME can last for a relative long time with an appropriate mass fraction of n-heptane. It proposes a way to change the evaporation rate of each component by altering the mass fractions in the DME/n-heptane mixture, in order to control the combustion of DME/n-heptane blended fuels.

1. Introduction

It is well-known that the performance of power generation systems is controlled by the vaporization process of fuel droplets [1]. Birouk et al. (2006) [2] stated that droplet evaporation involving heat and mass transfer processes are essential for engineering applications, such as the atomization, evaporation and combustion of liquid fuels in internal combustion (IC) engines, liquid-fueled rocket engines, gas turbine engines, as well as in liquid-fueled industrial burners. In those applications, the liquid fuel undergoes several processes before its gasification, which then mixes with the oxidant and burns to release energy. Spray, which can be treated as a cloud of droplets, may be generated through disintegration of a liquid jet issuing from various atomizers [3]. In the far field of the injector tip, a dilute region of more uniform size droplets might form [4]. The aerodynamic transport of droplets is dominant in the dilute dispersed spray region, and the droplet vaporization rate is the controlling factor for combustion in spray combustion systems. The overall rate of evaporation depends mainly on the temperature, the pressure, volatility and size of the droplets; and the relative velocity between the droplets and its surrounding gaseous medium. In practice, the evaporation and combustion of single droplets are essential in understanding spray flows that are generated commonly in liquid- fueled combustion systems. Such processes have been investigated widely in the last century, and the knowledge gained from these researches can be used to advance the understanding of the complex mechanisms of two-phase spray combustion phenomena encountered in liquid fueled combustors. Improving the efficiency of these systems requires a good understanding of the physics and chemistry of the complex interaction mechanisms between the liquid phase and the gas phase. Several attempts have been made to gain an understanding of the spray combustion problem, by isolating and studying a single droplet or an array of droplets of pure or multi-component liquids; see for example of Law [5] and Sirignano [6], and references cited therein. A single droplet is convinced to build an ideal model of the dilute region of the spray flow.

DME (Dimethyl ether) has been related to the reduction of emissions from diesel engines, especially with regard to the

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particulate emissions [7]. With the concerns of the decreasing petroleum reserves, DME is gathering more attention as an excellent alternative to diesel [8]. Compared to conventional diesel, the advantages of DME include reduced emissions of NO_x, soot, hydrocarbons and carbon monoxide. DME fueled CIDI (compression-ignition direct-injection) engines also generate less noise than conventional diesels [9]. With the increasing concerns on alternative fuels, it is essential to understand the effect of their different physical properties on combustion processes [10]. Law [5] proposed two models to describe the combustion of multi-component droplets, and he found that the components evaporated approximately sequentially in the order of their relative volatilities. Kim et al. [11] studied the effect of ambient pressure on the evaporation of a single droplet of n-heptane. They stated the evaporation of a spray could be explained by the atomization and evaporation of a single droplet. Li et al. [12] mentioned that evaporation played an essential role in the mixture formation and the combustion process of direct injection gasoline engines. Ji et al. [13] experimentally proved that starting a spark-ignited (SI) engine with pure DME could improve the combustion and emissions performance. Lu et al. [14] experimentally demonstrated the simultaneous reductions of NOx and soot using a dual-fuel sequential combustion, on a single-cylinder engine. Brenn et al. [15] proposed a multi-component model combined with UNIFAC (Universal Functional Activity Coefficient) approach, and investigated the evaporation characteristics of five-component droplets of ethanol, methanol, 1-butanol, n-heptane and n-decane. Ju et al. [10] investigated the effect of mass fractions on evaporation of a DME/n-heptane droplet at IC engine conditions, with the combination of UNIFAC method [15,16] and the non-equilibrium evaporation law [17,18]. Wang et al. [19] analyzed the evaporation characteristics of a multi-component droplet consisting of n-heptane, n-dodecane and n-hexadecane. They stated the finite evaporation rates of each component significantly affect local vapor concentrations which contribute a lot for the chemical kinetics of combustion. Therefore, the comprehensive modeling of the spray combustion in the IC engine requires an evaporation model to predict the vaporization characteristics of fuels and the local concentration of vapor phase of the fuel.

In the present work, to understand the interactive effect between DME and n-heptane on the evaporation of a bi-component droplet, a series of comparative analysis has been carried out for DME/n-heptane fuels with different droplet sizes at various internal combustion engine conditions. The scientific importance of the research is to discuss the evaporation characteristics of “each component” of DME/n-heptane droplets with different mass fractions at different conditions, and to find how the two main competing factors (the consumption of latent heat for evaporation and the heat transfer into the droplet) affect the evaporation behaviors of each component.

2. Physical and numerical models

The evaporation of multi-component droplets is fundamentally governed by the volatility differences among the components and liquid-phase mass diffusion. During the vaporization period, the internal compositions of the droplet vary in time, leading to the change of droplet temperature. These variations can be further affected by external convection due to the relative motion of droplets. The presence of large concentration gradient within the droplet interior for components of vastly different boiling points, as in the case of DME/n-heptane droplet, homogeneous nucleation could also occur, resulting in instant fragmentation of the droplet. However, in this paper, only high ambient pressures (31~51 bar) and small droplets (the diameters of which are less than 50 μm) are considered, therefore the effect of nucleation and boiling inside the droplet is ignored. It is assumed both thermal diffusivity and species liquid diffusion coefficient were finite, the temperature and the concentrations were uniformly distributed within the droplet [18]. With concerns to characterize the evaporation characteristics of the two-component droplets consisting of DME and n-heptane, a multi-component evaporation model (proposed by Brenn et al. [15]) combined with non-equilibrium law (proposed by Bellan et al. [20]) is implemented here. The liquid phase is treated as a thermodynamically ideal fluid, using the UNIFAC method [15] for calculating the component activities, and the gas phase is treated as ideal. The model had been validated for the evaporation of DME/n-heptane droplet in the previous work [10]. The properties of structure groups in different molecules of DME and n-heptane can be referred to the literature [10,16,21–23] and references cited therein.

2.1. Evaporation rate of and heat transfer rate of a multi-component droplet

The evaporation rate of a multi-component droplet is the sum of all component evaporation rates for an N-component mixture, as expressed in Eq. (1) [15].

$$\dot{m} = \sum_{i=1}^{N} \dot{m}_i = 2\pi \sum_{i=1}^{N} r_{V,i} \left(\overline{\rho D}_i\right)_g Sh_i^* \ln\left(1 + B_{M,i}\right) \tag{1}$$

where $\dot{m}_i$ is the evaporation rate of the component i in the droplet. $r_{V,i}$ is the volume equivalent partial radius of component i corresponding to its transient volume fraction ϕ_i in the liquid mixture, which is defined as $r_{V,i} = r\phi_i^{1/3}$ where r is the radius of the droplet. $\overline{D}_i$ is the mean diffusion coefficient of the vapor of component i in dry ambient gas. The modified Sherwood number Sh_i^* is calculated individually for each component i.

The heat transfer rate into a multi-component droplet is calculated for all components individually, as described in Eq. (2) [15].

$$Q_L = \sum_{i=1}^{N} \dot{m}_i \left[\frac{\overline{c_{p,i}}(T_\infty - T_d)}{B_{T,i}} - h_{fg,i}(T_d) \right] \tag{2}$$

where $h_{fg,i}(T_d)$ is the latent heat of evaporation of the liquid and B_T is the Spalding heat transfer number of component i.

2.2. Modeling the component activities in liquid mixtures by UNIFAC approach

Reid et al. [21] proposed to use Universal Functional Activity Coefficient (UNIFAC) method to calculate the activity coefficients of the component in the multi-component mixture. UNIFAC is a combination of the UNIQUAC method with solution-of-groups concept [21]. The UNIQUAC equation often gives good representation of vapor–liquid equilibrium for multi-component mixtures [21]. The UNIFAC model contains a combinatorial part, essentially due to differences in size and shape of the molecules in the mixture, and a residual part, essentially depends on group areas and group interaction. Brenn et al. [15] compared numerical results to the experimental data, and the model with UNIFAC method represented better approach than the one with Wilson's coefficient.

The mass fraction $Y_{eq,i}$ of the vapor component i at the surface of an equilibrium state can be calculated from its mole fraction$x_{eq,i}$ and its activity coefficient of the component in the multi-component liquid mixture, as expressed in Eq. (3) [15].