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Numerical simulation of droplet evaporation characteristics of multi-component acetone-butanol-ethanol and diesel blends under different environments

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ABSTRACT

Effects of ambient temperature, pressure and relative velocity between droplet and airflow on evaporation characteristics of multi-component droplet were investigated numerically. A recently proposed multi-component model was adopted in the present study by considering the pressure effects. The result shows that, present model predicts satisfactory results when compares with experimental data. Increasing ambient temperature especially promotes evaporation of low volatile components in ABE20. Ambient pressure influences ABE-diesel blends droplet evaporation differently under various ambient temperatures. For low ambient temperature environment, droplet evaporation rate decreases with ambient pressure increasing, especially for low diffusion coefficient components. However, evaporation characteristic shows an opposite tend under high ambient temperature environment, where evaporation rate increases with ambient pressure increasing. Additionally, increasing ambient pressure promotes maximum evaporation rate of high diffusion coefficient components. With temperature increasing, this promotion extends to low diffusion coefficient components. Finally, increase relative velocity between liquid and gas phase substantially enhances evaporation of high diffusion coefficient components in the mixture.

1. Introduction

The interest in alternative fuel of diesel engine has been mainly stimulated by depletion of fossil fuels and the need to control climate change caused by carbon dioxide emissions. Butanol is considered as a favorable alternative fuel for diesel because of it superior properties [1,2]. However, butanol is generally produced by distilling acetone-butanol-ethanol (referred to as ABE hereinafter), which is costly and requires extra energy. Directly use ABE can save enormous expenses and be more energy saving [3]. For this reason, the probability of ABE directly using as renewable fuel has been studied for a long time. To investigate the combustion characteristics and emission performance of ABE-diesel blends, Zhou et al. [4] experimentally studies the combustion of ABE-diesel blends in a constant volume chamber. Wu et al. [5,6] experimentally investigated the spray combustion characteristic of ABE and diesel by using forward illumination light extinction technology. These studies demonstrate that ABE-diesel blends possess good combustion characteristics and emission performance.

ABE-diesel blends consist of many components and the volatility differences of each fuel components are large. In order to improve combustion and emission performance of ABE-diesel blends, the evaporation experiments of ABE, diesel and their blends droplets under varying ambient temperatures so to investigate the evaporation characteristics of multi-component droplets were conducted, in one of our previous publication [7]. The results show that, droplet lifetime differences of ABE and diesel decreases with increasing ambient temperature. In addition, bubble formation and rupture, which was resulted from the trapping of high volatile components in droplet by low volatile components near the surface, were observed in the fluctuation evaporation stage. Effects of ABE content on evaporation of ABE-diesel blends were investigated by numerical method to further analyze droplet evaporation characteristics [8]. The established multi-component evaporation model was subsequently validated by experimental results. The results show that the bubble formation could be observed when droplet temperature exceeds boiling temperature of low volatile components. In addition, the timing of internal gasification and internal gasification intensity were related to the ABE content. As previous studies [7,8] indicated, evaporation characteristics of ABE-diesel droplet are relevant to fuel properties and ambient environment conditions. It should be noted that, the surround environment in internal combustion engine combustion chamber is complicated and characterized by high temperature, high pressure and intense turbulence.

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Nomenclature

$\dot{m}_d$	evaporation rate (kg/s)
r_s	droplet radius (m)
ρ	Density (kg/m^3)
D	diffusion coefficient (cm^2/s)
sh	Sherwood number
B	Spalding number
Nu	Nusselt number
k	thermal conductivity (W/m·k)
c_p	specific heat (J/(kg/K))
$L(T)$	latent heat (J/kg)
F	Stefan correction factor
$\dot{Q}_l$	Liquid-phase absorption heat (W)
Y	mass fraction
X	molar fraction
M	molar mass
$\dot{q}_r$	fiber conduction heat (W)
$\dot{q}_f$	thermal radiation heat (W)
T	Temperature (K)
χ	correction factor
Pe	Peclet number
Re	Reynolds number
Sc	Schmidt number
γ_i	activity coefficient of species (i)
ω	acentric factor
D_{AB}	diffusion coefficient of component A in component B
M_{AB}	average molar mass
t	Time (s)
R	gas constant
p	Pressure (Pa)

Subscripts

v	vapor
s	surface
∞	ambient conditions
M	related to mass transfer
T	related to heat transfer
g	average parameters of vapor mixture
ref	reference state
0	initial
l	liquid
eff	effective
i	index for individual species
amb	ambient
c	critical

Therefore, it is essential to fully understand the effects of environment conditions on evaporation characteristics of ABE-diesel blends droplet by establishing a multi-components model considering the variation of ambient conditions.

The evaporation process of multi-component fuel droplet had been extensively studied in the recent years. Liu et al. [9] numerically studied the influence of environmental pressure on evaporation characteristics of decane-ethanol bi-component droplet by developing a multi-component evaporation model. The results indicate that temperature characteristics of droplet vary in different ambient pressures. In addition, the concentration of ethanol has different effect on droplet evaporation in different evaporation phases. Saha et al. [10] investigated the evaporation process of diesel and biodiesel blendes in high temperature convective environment which is closer to the real evaporation conditions by proposing a multi-component evaporation model. The results reveal that increasing biodiesel content in the blends increases droplet lifetime time and final surface temperature. Gavhane et al. [11] investigated the influences of droplet constituent compositions on evaporation by two different fuel droplets, one droplet compositions with widely varying volatility and another with close volatility. The results show that the heavier component in droplet tends to control droplet temperature history, however the mass depletion histories are related to the difference between different droplet components. Manjunath et al. [12] experimentally investigated the vaporization characteristics of diesel and biodiesel blend fuels by using droplet suspension method. The results show that increasing diesel content in biodiesel-diesel blends reduces the overall vaporization time due to the higher volatile of diesel. These studies show that the fuel properties significantly influence the evaporation characteristics of multi-component droplet, however, the evaporation characteristic affected by complicated ambient conditions such as the coupling effect of ambient temperature, pressure and relative velocity has been barely studied.

For non-ideal multi-component mixtures such as ABE-diesel blends, due to the large polarity difference between two components (i.e., diesel and ABE), non-ideal vapor-liquid equilibria substantially influence the droplet evaporation characteristic [13,14]. Consequently, the non-ideal phase equilibrium behavior must be considered by using an activity coefficient. Several researches have applied activity coefficient to describe non-ideal phase equilibrium behavior, and obtain satisfactory results [14–16]. In addition, duo to the significant gas molecules interaction under high ambient pressure, gas effect plays an increasingly important role in influencing droplet evaporation characteristics [17,18]. Consequently, we implemented the gas effects in the model so as to accurately simulate the fuel evaporation characteristic. Zhu et al. [19] studied droplet evaporation by using three different equations (i.e., Peng-Robison, Redlich-Kwong (RK) EOS and Soave-Redlich-Kwong (SRK) EOS equation), the results show that the Peng-Robinson equation predicts satisfactory result under a wide range of ambient pressures.

The present study aims to analyze the evaporation characteristics of multi-component droplet under different ambient conditions. Since diesel is represented by six components, a nine component evaporation model for ABE-diesel blends droplet which accounts for all features mentioned above, including the use of Universal Functional Activity Coefficient (UNIFAC) method to describe molecular structure difference between ABE and hydrocarbons. We shall employ PR EOS to represent the real gas effect under high ambient pressure. The simulation model shall be validated with experimental results in droplet evaporation. In addition, influences of ambient temperature, pressure and the relative velocity between droplet and airflow on evaporation characteristics of multi-components single droplet will be presented in this paper.

2. Models

2.1. Assumptions

The suppositions of the numerical model are as follows: (1) the droplet is symmetric, which is reasonable for small droplets [20]. For the case in our paper, droplet diameter is 50 μm, so it can be treated as spherical symmetric; (2) the temperature and composition of droplet are uniform but vary with time, which is suitable for one-dimensional liquid phase calculation; (3) as the thermal diffusivity of gas phase is greater than liquid phase, the gas phase surrounding the droplet is in quasi-steady state; (4) both gas and liquid phases are at thermodynamic equilibrium at the surface of droplet; (5) the gas mixture surrounding the droplet is insoluble in liquid phase. Droplet can not reach critical state under present ambient environment with temperature region from