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An enhanced multi-component vaporization model for high temperature and pressure conditions

Wuqiang Long, Ping Yi, Ming Jia *, Liyan Feng, Jingchen Cui

Institute of Internal Combustion Engine, School of Energy and Power Engineering, Dalian University of Technology, PR China

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ABSTRACT

An enhanced multi-component vaporization model was proposed to simulate the vaporization process of fuel droplets under high ambient temperatures and pressures. In the present model, the heat flux of conduction, enthalpy diffusion, and radiation absorption in the gas phase are calculated by Fourier's law, the multi-component diffusion sub-model, and a simplified analytical solution of the radiative heating, respectively. A surface temperature sub-model was employed to evaluate the average temperature within the droplet and the surface temperature of the droplet. For calculation of vapor–liquid phase equilibrium, a real and an ideal gas approach was used for high and low ambient temperatures and pressures, respectively. Moreover, the dependence of gas physical properties on temperature and pressure is also considered. Based on the enhanced vaporization model, extensive verifications for different multi-component droplets were conducted, and the results indicate that satisfactory agreements between the predictions and measurements can be achieved. Finally, the multi-component vaporization model was applied to investigate the vaporization characteristics of practical fuel droplets with a wide range of diameters at high ambient temperatures and pressures, and the effects of radiation absorption and real gas behavior on the vaporization process were understood. It is found that the influence of radiation absorption on the vaporization behavior strongly depends on the droplet diameter and the ambient temperature, and the effect of ambient pressure on the average vaporization rate is determined by the ambient temperature. Considering the compromise between computational accuracy and efficiency, a pressure criterion (P') was introduced for the choice of ideal or real gas approaches, and a diameter criterion (D') was also defined to decide whether to consider the radiation absorption in the vaporization model.

1. Introduction

Accurate modeling of droplet heating and vaporization is essential for the simulation of the combustion process of liquid fuel in practical devices [1]. Since the components in practical fuels are very complicated, employment of the multi-component vaporization model is important to achieve highly accurate predictions. Recently, many multi-component vaporization models have been proposed [2].

As encountered in many practical applications, such as gas turbines and diesel engines, the influence of ambient pressure on the fuel vaporization rate should be taken into account. In previous works, with the consideration of computational efficiency, the Rault's law has been widely used to estimate the vapor pressure of mixture based on the simplification of the vapor–liquid phase equilibrium under low ambient pressures [3]. Since the assumption of the vapor–liquid phase equilibrium could lead to large deviations at high pressures, the real gas behavior, the solubility of the ambient gas into the liquid droplet, and the equality of the fugacity of each species are markedly important [4]. The studies on the droplet vaporization at high ambient pressures have been conducted by many researchers [4,5]. Hohmann et al. [5] proposed the vaporization model with real gas behavior, and it was found that the predictions were consistent with the experimental data on the droplet vaporization rate at high ambient pressures. However, the above two models are limited to single-component fuels.

Recently, Aggarwal et al. [6] employed the multi-component vaporization model with real gas behavior to simulate the vaporization characteristics of the multi-component droplets under high ambient pressures, whereas the history of droplet size was not validated by the experimental data for binary or multi-component droplets under high ambient pressures. To include the non-ideal behavior in the gas phase and the gas solubility at the droplet

* Corresponding author.

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Nomenclature

A_i, B_i, C_i	empirical coefficients in Eq. (16)
$B_{i,\lambda}$	Plank function
B_m	spalding mass transfer number
C_1, C_2	constants in Eq. (8)
c	specific heat
D'	diameter criterion
$D_{i,g}$	diffusion coefficient
D_0	droplet diameter
E_{im}	computational efficiency
H	latent heat of vaporization
h_i	specific enthalpy
$k_{i,\lambda}$	index of absorption
M	molecular weight
$\dot{m}$	mass vaporization rate
N	total number of species
n_i	refractive index
P	pressure
P'	pressure criterion
P_R	radiation intensity
$\dot{Q}_{conduction}$	conduction heat flux
$\dot{Q}_{enthalpy}$	enthalpy diffusion heat flux
$\dot{Q}_{gas}$	total heat flux from ambient gas
$\dot{Q}_{droplet}$	heat flux penetrated into droplet
$\dot{Q}_{radiation}$	radiation absorption heat flux
$Q_{i,a}$	efficiency factor of absorption
R	droplet radius
R_g	gas constant
T	ambient temperature
t	time
t_d^w, $t_d^{w/o}$	droplet lifetime
u	velocity of ambient gas
u^c	corrected velocity
x	mole fraction
y	mass fraction
v	diffusion velocity
Z	compressibility factor

Greek symbols

ρ	density
λ_g	thermal conductivity of gas
λ_i	wavelength of absorption
$\varphi_{i,j}$	binary interaction coefficient in Eq. (20)
ϕ_i	fugacity coefficient
φ_p	constant in Eq. (31)
ε	convergence criterion
ω_i	acentric factor
$\Delta\dot{m}_{ave}$	difference in average vaporization rate
Δt	time step

Subscripts and superscripts

ave	average
b	boiling
d	within the droplet
f	reference coefficient
g	in the ambient gas
i, *j*	species
ideal	ideal gas approach
nb	normal boiling
r	reduced coefficient
real	real gas approach
s	at the droplet surface
v	vapor
w	with considering radiation
w/o	without considering radiation

surface, the Peng–Robinson equation and van der Waals mixing rule have been widely applied for the high ambient pressures [7,8]. It is found that, as the Peng–Robinson equation and van der Walls mixing rule are employed, the interaction coefficients between the binary components have crucial effects on the prediction of vaporization rate, which makes the vaporization of binary or multi-component droplet significantly different from that of single-component droplet.

On the other hand, in previous multi-component vaporization models under high ambient pressures, the gas-phase diffusion coefficients of different species are assumed to be equal, and the enthalpy heat flux due to species diffusion is neglected. These simplifications could introduce significant discrepancies between the predicted vaporization rate and the measurements [9]. Therefore, for a more realistic description of the vaporization of multi-component fuels, it is necessary to consider the effects of multi-component diffusion coefficients. This consideration is simplified as multi-diffusion sub-model in this study.

Because fuel droplets are exposed to high-temperature surroundings, the study of the vaporization rate under high ambient temperatures should be addressed for the simulations in practical engines, in which the fuel droplet can be simultaneously heated by the conduction and radiation absorption from the hot ambient gas or hot external flame [1]. The effects of high ambient temperature on the temperature distribution within the droplet have been investigated [10]. However, only a few studies focus on the effects of thermal radiation absorption from the hot ambient gas on the droplet vaporization rate. In the work of Abramzon et al. [11], the radiation absorption was considered to investigate the vaporization process of n-decane and diesel droplet under high ambient temperature conditions. The results showed that the radiation absorption had a more pronounced effect on the vaporization history of a diesel droplet than that of an n-decane droplet. This could be attributed to the difference in the number of C—H bond for the two test fuels [12]. However, the model of Abramzon et al. [11] is only limited to single-component droplets, and the diesel was represented by n-dodecane in their simulation.

For the high ambient temperature conditions, the heat and mass transfer within the droplet during the vaporization process have also been extensively studied [13]. Aggarwal et al. [14] compared the infinite-diffusion model and diffusion-limited model for the stagnant droplet vaporizing under high temperatures and pressures. It was found that the vaporization curve for these two models are very similar. At the same time, Aggarwal et al. [15] found that the predicted vaporization behavior is significantly more sensitive to the droplet heating than the component distribution within the droplet. This is because that the mass transfer rate of the fuel components is much larger than the heat transfer rate within the droplet [16].

In the previous vaporization models, the sub-model of heat transfer in the liquid droplet can be classified into three categories, i.e., infinite conductivity model, finite conductivity model, and vortex model. In the infinite conductivity model, it is assumed that no temperature gradient exists in the droplet interior, which could lead to some deviations on the predicted droplet temperature and vaporization rate [2]. The finite conductivity model considers the