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Development of a quasi-dimensional vaporization model for multi-component fuels focusing on forced convection and high temperature conditions

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ABSTRACT

A new quasi-dimensional multi-component vaporization model considering the finite thermal conductivity and mass diffusivity within the droplet was constructed. First, the heat flux of conduction, enthalpy diffusion, and radiation absorption in the gas phase were calculated based on the Fourier's law, a multi-diffusion sub-model, and a simplified analytical solution, respectively. The phase equilibrium at the gas–liquid interface was calculated by the ideal and real gas approaches according to the ambient pressure. For the liquid phase, the assumption of the quadratic polynomial distributions of the temperature and component concentration within the droplet was proposed in the quasi-dimensional model. Then, the proposed vaporization model was extensively validated by the experimental measurements, and good agreements were observed. Based on the computational results, the vaporization and movement behaviors of fuel droplets under forced convection conditions were further understood. Finally, by comparing with the zero-dimensional vaporization model with uniform temperature and component concentration distributions within the droplet and the one-dimensional vaporization model with finite thermal conductivity and mass diffusivity in the radical direction of the droplet, it is found that the quasi-dimensional model agrees better with the one-dimensional model than the zero-dimensional model, especially for the conditions with high ambient temperature and velocity. Sensitivity analysis indicates that the temperature gradient within the droplet plays a significantly important role in the droplet vaporization process.

1. Introduction

In internal combustion engines, fuel droplets vaporize under a wide range of ambient temperature, pressure, and convection conditions [1]. Many vaporization models have been proposed to predict the droplet heating and vaporization processes under engine-relevant conditions. It has been found that the droplet vaporization rate under the convection conditions significantly deviates from the classic D^2 vaporization law due to the high Grashof number and Reynolds number [2]. Moreover, because most of practical liquid fuels are inherently multi-component, the single-component vaporization model cannot accurately capture the temporal evolutions of the droplet diameter and the vaporization behavior of each component in the fuel. Hence, there is a need to develop a reliable model to predict the vaporization processes of multi-component droplets focusing on forced convection conditions.

In practical engines, the in-cylinder ambient conditions considerably vary with the combustion modes and the operating conditions. During the cold start of engines, the ambient temperature and the relative velocity between ambient gas and droplet are relative low, and the highly volatile components in the fuel play an important role in the ignition and burning processes. Due to the low droplet temperature, the mass diffusivities of the liquid fuel are low, which leads to the high gradient of the component concentration within the droplet [3]. On the contrary, in the conventional diesel combustion with the injection timing around top dead center (TDC), the fuel droplets vaporize in high ambient temperature and forced convective conditions. The rapid consumption of the light components at droplet surface results in the high gradient of component concentration within the droplet [4], although the diffusion coefficient of the liquid fuel is large at high temperatures. In addition, because of the high ambient temperature and the high vaporization rate, the temperature gradient near the droplet surface is very large. Therefore, the vaporization model needs to account for the gradients of the temperature and component

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Nomenclature

a, b, c	constants in Eqs. (10) and (15)
$A_{i,p}, B_{i,p}, C_{i,p}$	constants in Eq. (32)
B_i	Plank function
B_h	heat transfer number
C_D	drag coefficient
D	diffusion coefficient
D_0	initial droplet diameter
E_i	efficiency factor of absorption
F_{acc}	computational error
F_{eff}	computational efficiency
g	gravitational acceleration
h_i	specific enthalpy
H_{latent}	latent heat of vaporization
k_i	index of absorption
$m_{i,l}$, m_l	mass
$\dot{m}_{i,l}, \dot{m}_l$	mass vaporization rate
N, N_l	number of species
Nu	Nusselt number
P	pressure
P_R	radiation intensity
Pe	Peclet number
$\dot{q}$	heat flux
R	distance from droplet center
$\lvert\dot{R}_l\rvert$	absolute vaporization rate
Re	Reynolds number
r	dimensionless radius
S	distance of droplet movement
Sc	Schmidt number
T	droplet temperature
t_1, t_2, t_3	moments of time
t_{cal}	calculation time
u	velocity
$v_{i,g}$	diffusion velocity
x	mole fraction
y	mass fraction

Greek symbols

ρ	density
λ	thermal conductivity
$\lambda_{i,1}, \lambda_{i,2}$	wavelength
ε_i	normalized fraction
ϕ_i	fugacity coefficient
ω_i	acentric factor

Superscripts

a	average
c	corrected
s	surface

Subscripts

i, j	species
g	gas
l	liquid
p	pressure
r	relative
re	reduced
ref	reference
v	vapor
0	initial values

concentration within the droplet during the vaporization process under engine-relevant conditions.

In the Computational Fluid Dynamics (CFD) simulation of practical engines, the zero-dimensional droplet vaporization model is usually utilized for saving the computational time, in which the temperature and component distributions are assumed to be uniform within the droplet. The limitations of the zero-dimensional model have been revealed under engine-relevant conditions by Bertoli et al. [5], thus the enhanced one-dimensional vaporization model was proposed. In most of the present one-dimensional vaporization models, only the temperature inhomogeneity is considered, while the stratification of the component concentration within the droplet is ignored. However, Brereton [6] found that the mass diffusivity of the liquid component also plays an important role on the droplet vaporization process, since the thermal energy and mass diffusion equations are closely coupled. Hence, it is necessary to clarify the importance of the component concentration gradients within the droplets on the vaporization behavior for multi-component fuels.

Although the benefits of the one-dimensional vaporization model have been widely acknowledged [5,7], it is still a challenge to be applied in CFD simulations owning to the extremely high computational cost [8]. In the one-dimensional vaporization model, solving the governing equations of energy and species in the liquid phase using implicit finite difference scheme along the radical direction occupies relatively long computational time, and the computational cost increases sharply with the increase of discrete layers and the decrease of time step [8]. Hence, construction of a vaporization model with consideration of the temperature and component concentration gradients within the droplet with minimal computational cost is highly demanded for engineering applications.

Great efforts have been made to improve the computational efficiency for modeling the droplet heating and vaporization processes [9,10]. Dombrovsky and Sazhin [11] used the parabolic temperature profile model with the presumed parabolic temperature distribution within the droplet to simulate the heat transfer process in the liquid phase for the single-component droplets. Ra et al. [10] developed a simplified surface temperature sub-model, in which the difference between the droplet surface and core temperatures is considered, thus the heat transfer within the droplet can be simulated. However, infinite mass diffusion, i.e., uniform concentrations of various components within the droplet, is assumed in the Ra et al. model [10]. On the contrary, Raghuram et al. [12] proposed a two-layer film theory to include both the finite thermal conductivity and mass diffusivity within the binary-component droplets. In their model, explicit expressions for the heat and mass transferred from the ambient gas to the droplet interface, as well as within the droplet, are derived from the quasi-steady energy and continuity equations. Using the unsteady equivalent boundary layer thickness, Abianeh et al. [13] extended the Raghuram et al. model [12] for multi-component droplets. In the work of Abianeh et al. [13], the thermal boundary layer thickness is described as $\delta_{thermal} = \sqrt{\pi \alpha t_\tau}$, and the mass transfer boundary layer is described as $\delta_{diffusion} = \sqrt{\pi D t_\tau}$, where t_τ is an empirical constant estimated based on the heat and mass transfer-limited integration time step. Thus, some deviations could be introduced under different engine-operating conditions.

Considering the compromise between the computational accuracy and efficiency for multi-component fuel droplets, a quasi-dimensional vaporization model is proposed in this study based