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Research Paper

An efficient liquid film vaporization model for multi-component fuels considering thermal and mass diffusions

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HIGHLIGHTS

- An quasi-dimensional multi-component vaporization model for wall film was developed.
- The thermal and mass diffusion in the film was described by high-order polynomials.
- Effect of the thermal and mass diffusion on diesel film vaporization was discussed.
- The relative error of various vaporization models for wall film was discussed.
- Computational accuracy and efficiency of models were evaluated in CFD application.

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ABSTRACT

An improved multi-component quasi-dimensional vaporization model for wall film was proposed with considering the finite thermal and mass diffusions within the liquid film. In the improved model, high-order polynomials were introduced to describe the profiles of the temperature and component concentrations within the film. The results show that the predictions from the present quasi-dimensional model agree well with those predicted by the one-dimensional model. By investigating the effect of the thermal and mass diffusions on the vaporization of the diesel film, it is found that the thermal diffusion plays a more dominant role in the multi-component film vaporization. Compared with the linear temperature model with the linear temperature and uniform component distributions in the film, the application range of the quasi-dimensional model is considerably wider and the computational error is significantly reduced. Finally, the linear temperature, quasi-dimensional, and one-dimensional models were integrated into a Computational Fluid Dynamics (CFD) code for the simulations of film vaporization in the flow over a backward facing step and in a practical diesel engine. The results indicate that the improved model gives much better agreement with the one-dimensional solutions than the linear temperature model, while maintaining high computational efficiency under different operating conditions.

1. Introduction

The vaporization and combustion of the wall film caused by the spray/wall interaction have attracted increasing interests for internal combustion engines, for example, diesel premixed charge compression ignition (PCCI) engines employed with early injection strategy and gasoline direct-injection (GDI) engines. When wall wetting phenomenon occurs, the characteristics of the wall film evolution and vaporization have remarkable influence on the fuel/air mixture, and then fuel economy and engine emissions. It has been found that the deposited wall film is responsible for the high soot emissions in GDI engines [1]. Fang et al. [2] pointed out that the slow vaporization of the wall film can lead to the “pool file” phenomenon, which results in the incomplete combustion and then high hydrocarbon (HC) emissions. Therefore, deep knowledge to the wall film heating up and vaporization processes will benefit the control of the harmful emissions and the improvement of engine efficiency.

It is still challenging to obtain reliable experimental data on the wall film vaporization process, especially under engine-relevant conditions due to the extremely small temporal scale ($t \sim o(\mathrm{ms})$) and spatial scale ($h \sim o(\mu\mathrm{m})$) involved. Alternatively, the wall film model can help to understand the film heating up and vaporization processes. Moreover, the single-component fuels are usually employed as the surrogate for practical fuels in engine simulations. However, the light-end components in gasoline and diesel vaporize

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Nomenclature

a_l	thermal diffusivity
a_0, a_1, a_2, a_3	constants in Eq. (8)
A	the highest order of the polynomial
A_0	area of the wall film
b_0, b_1, b_2, b_3	constants in Eq. (11)
B_M	Spalding mass transfer number
c_l, c_p	specific heat capacity
D	diffusion coefficient
H_l	latent heat of vaporization
h_t	heat transfer coefficient
h_y	mass transfer coefficient
L_c	characteristic length
N_l	number of species
Nu	Nusselt number
P	pressure
$P_{i,v}$	saturated vapor pressure of species i
Pr	Prandtl number
$\dot{q}_{in}$	gas/film heat flux
Re	Reynold number
Sc	Schmidt number
T	temperature
u^*	friction velocity
V_g	gas velocity
V_{in}	inlet velocity
x	mole fraction
Y	mass fraction
y^+	dimensionless normal coordinate
z	z-coordinate
Z	compressibility factor

Greek symbols

δ	film thickness
ε_i	normalized fraction of fuel vapor
λ	thermal conductivity
μ	viscosity
ρ	density
τ	time
φ_{ij}	binary interaction coefficient
ϕ	fugacity coefficient
$\dot{\Phi}$, $\dot{\Phi}_i$	vaporization rate
Ψ	a parameter defined as $\Psi = \frac{\dot{\Phi}(Y_{i,l,s}-\varepsilon_i)}{\rho_l D_{i,l}}$
Ω	a parameter defined as $\Omega = \delta \cdot \dot{q}_{in}/\lambda_l$
ω_i	acentric factor

Subscripts

i, j	species index
g	gas
l	liquid
m	mean
s	surface
v	vapor
0	initial value

preferentially, and significantly affects the global vaporization behavior of the wall film, which cannot be reproduced by the single-component fuel model.

Two methods exist for multi-component fuel model, namely, the continuous multi-component (CMC) method and the discrete multi-component (DMC) method. The multi-component fuel is represented by a probability distribution function (PDF) on the basis of a related parameter, such as the component molecular weight [3] in the CMC method. The CMC model can effectively reduce the computational time while maintaining the capabilities to describe the complex compositions of practical fuels, whereas it cannot be directly integrated with the combustion simulations with detailed chemistry [4]. In the DMC method, limited discrete components were chosen to model the fuel. Although practical diesel and gasoline contain hundreds of hydrocarbons, their vaporization characteristics can be satisfactorily reproduced with several representative components [5]. In addition, the DMC model can be coupled with the chemical mechanism to simulate the combustion process.

For PCCI engines, the wall film is unavoidably formed owing to the fuel injection in the early compression stroke and the low volatility of diesel. As the compression stroke continues, the temperature and the relative velocity between the charge and the wall film increase within the cylinder, so the wall film is heated up by the piston wall and the ambient gas simultaneously. At the same time, the highly volatile components in the liquid film rapidly vaporize at the film surface, leading to large gradient of the component concentrations within the liquid film. Therefore, the temperature and component concentrations gradients in the film interior should be considered under the conditions with high vaporization rate.

At present, the wall film heating up and vaporization models available in the literature can be classified into four types. The first type is the zero-dimensional model, in which the finite thermal and mass diffusions are neglect (infinite diffusion), and the average temperature and mass concentration of each species in the film are obtained based on the energy and mass conservations, respectively. O'Rourke and Amsden [6] extended the zero-dimensional film model for single-component fuels with the consideration of the temperature difference between the internal film and the liquid film surface (referred as the linear temperature model in this study). The O'Rourke and Amsden model [6] has been widely adopted in CFD codes owing to its high computational efficiency. However, unneglectable error can be produced under engine-relevant conditions, which will be discussed in detail in the following study.

The second type is the one-dimensional model, in which the stratifications of the temperature and the mass fraction of each species in the liquid film are taken into account. Torres et al. [7] proposed a one-dimensional vaporization model for the wall film by discretizing the interior of the wall film into nearly 10 nodes. The results demonstrate the importance of the thermal and mass diffusions within the liquid film on the evolution of the wall film vaporization. However, it is still a challenge to adopt the one-dimensional film model in multi-dimensional CFD simulations due to its low computational efficiency, especially when a large amount of components are involved.

Moreover, by directly solving the energy equation of the wall film, Yan et al. [8] and Song et al. [9] proposed analytical solutions of the temperature within the film. However, only the single-component fuel is considered for simplicity. Moreover, the transcendental equations must be solved numerically in order to obtain the analytical solutions, occupying much computational time, which prohibits its application in CFD modeling.

The last type of the wall film model is the quasi-dimensional model, in which the distributions of the temperature and the component fraction of each species in the wall film are described by presumed profiles. Compared with the one-dimensional model