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An analogical multi-component vaporization model for single diesel droplets

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ABSTRACT

An analogical multi-component (AMC) vaporization model for diesel droplets was proposed and constructed. First, sensitive properties, which varied with components show significant effects on the vaporization behaviors, were determined, including the liquid density, vapor pressure, enthalpy of vaporization, and gas diffusivity. In the AMC model, the diesel droplet is assumed to be modeled as a single quasi-component, which is based on the introduction of a reference component and two dimensionless analogies, the property and vaporization rate analogies. The property analogy was defined as the ratio of properties of each component to those of the reference one, and the vaporization rate analogy was estimated based on the mass transfer number. Then, the proposed AMC model was extensively validated by experimental results, and good agreements were obtained. In order to evaluate the performance of the AMC model, a discrete multi-component (DMC) model, in which diesel is described by several components, and a sequential multi-component (SMC) model, in which the diesel was represented by a varied single component with the vaporization progressing, were carried out. Extensive comparisons of the AMC, SMC, and DMC models in the aspects of computational accuracy and efficiency were performed. It is found that the AMC model not only could improve the computational efficiency compared with the DMC model, but also illustrates significantly better accuracy than the SMC model under the conditions tested in this study.

1. Introduction

The combustion phenomenon has been widely used in many applications, and the fuel spray penetration has plays an important role among all stages of combustion processes. Accurate predicting the droplet vaporization process and corresponding flow evolutions, therefore, is important since it straightly influence the onset of combustion [1]. In previous studies, numerous models have been carried out for single fuel droplets, and most of these models have been typically incorporated into multidimensional CFD codes where droplet vaporization processes are modeled alongside the chemical processes in realistic enclosures. The complexity of the involved phenomena is in a necessary of a compromise between the accuracy and efficiency of the models [2,3]. In practice, most developed vaporization models [4–8] were based on some assumptions, including: (1) the diesel is approximated by a single component; (2) the thermal and transport properties are estimated by simple empirical formulas; (3) the phase equilibrium at gas-liquid interface was described by ideal gas method; (4) the gradient of temperature and species concentration in droplet was ignored; (5) the deformation of droplet in forced convections was not considered. Some of these assumptions have been relaxed in previous works [7–10], and the most prominent assumption is that the diesel is substituted by a single component [11,12]. Stagni et al. [13] found that the volatile component makes a pronounced influence on the ignition time through a multi-component model. Thereby, a new solution was proposed in this study to describe the composition distribution in the multi-component diesel droplet.

The multi-component vaporization models can be classified into four types, i.e., discrete multi-component (DMC) [14,15], continue multi-component (CMC) [16,17], hybrid multi-component (HMC) [8], and multi-dimensional quasi-discrete (MDQD) [18] approaches. In the DMC approach, the fuel is assumed to be composed by a finite number of components, and each component can be well tracked by solving the transport equations. This approach is widely applicable but limited in the cases where a small number of components are considered. As an alternative, in the CMC approach, the fuel composition is characterized by a continuous probability density function (PDF). This approach shows significant advantages in terms of computational efficiency, however, the deficiency is that this approach limits the accurate prediction of each component. Taking into account the advantages and disadvantages of DMC and CMC approaches, the HMC approach was proposed in which each group of hydrocarbon in diesel is described by a

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Nomenclature

a_i, b_i, a_{ij}	Parameters in PR EoS
c_i	Corrected volume
A, B, C	Empirical constants
B_m	Mass transfer number
$D_{i,j}$	Binary diffusion coefficient
D	Droplet diameter
Gr	Grashof number
h	Specific enthalpy
H	Enthalpy
$K_{\overline{phy}}$	Predicted vaporization rate
L_{ev}	Latent heat of vaporization
M	Molecular weight
$\dot{m}$	Mass vaporization rate
m_i	Parameter in PR EoS
N	Number of species
$N_{i,C/H/ring}$	Number molecular group
Nu	Nusselt number
P	Pressure
Q	Heat flux
r	Normalized diameter
R	Droplet radius$g$
R_g	Gas constanti,j,k
Re	Reynolds number
$R_{j,\rho}$, $R_{j,L}$, $R_{j,D}$	Analogies of properties
$R_{j,\dot{m}}$	Analogies of vaporization rate
Sc	Schmidt number
Sh	Sherwood number
$t_{\overline{phys}}$	Predicted heating time
T	temperature
u	Velocity of mixture
v	Diffusion velocity
V	Volume
x	Mole fraction
y	Mass fraction
Z	Compressibility factor

Greek symbols

α_i	Parameter in PR EoS
ρ	density
λ	Thermal conductivity
ω	Acentric factor
ϕ	Fugacity coefficient
ε	Normalized fraction

Subscript

B	Base component
bo	Boiling property
c	Critical property
g	Gas
i,j,k	Component
l	Liquid
r	Reduced property
s	Droplet surface
v	vapor

separated PDF. The HMC approach shows satisfactory compromise between the accuracy and efficiency, but it is limited to the utilization of ideal gas equation of state at present [8]. Alternatively, in the MDQD approach, the fuel composition is modeled as a few quasi-components with non-integer numbers of carbon atoms, and this method shows a great advantage in computational efficiency and accuracy compared to the traditional DMC model with large number components [18].

It is noted that there are a lot of repetitive and alternative calculation steps in the determination of properties and vaporization rate for each component in previous multi-component vaporization models, consequently resulting in the computationally expensive compared to the single component model, in which a single component was selected to represent the realistic fuels. Focus on this deficiency, an analogical multi-component (AMC) model utilizing a single quasi-component based on the introduction of one reference component and two dimensionless analogies is proposed, in which the influence of the properties varied with components on the vaporization behaviors need to be adequately understood.

Sazhin et al. [19,20] and Pitz et al. [21] have pointed out that the accuracy of the vaporization model is strongly dependent on the evaluation of thermo-physical properties. Most studies in the literature were focused on the influence of the thermo-properties varied with temperature and pressure on the vaporization behaviors, including the non-ideal behaviors in the gas and liquid phases. It is found that, however, the detailed effects of the properties varied with different components on the model accuracy have not been well understood, even though the vaporization characteristics of multi-component droplets have been extensively studied. Thereby, it is necessary to analyze the influence of the properties varied with components on the vaporization behaviors, and determine the sensitive properties varied with components in the vaporization model.

In previous vaporization models taking into account the influence of high pressure on the vaporization behaviors, some thermo-properties are still approximated using the ideal empirical formulas, only with respect to the molecular groups, correlating equations, and the transient temperature [22]. However, the ideal empirical approach is difficult to accurately predict non-ideality behaviors of fluids under high pressures. Thus, the non-ideal approach, such as the Peng-Robinson (PR) equation of state (EoS) [23], need to be used. Due to the low computational efficiency of PR EoS, it is difficult to apply it to predict all thermo-properties for multiple components in practical spray applications. In order to consider the compromise between the computational accuracy and efficiency, a detailed sensitive analysis need to be performed to study the dependence of temperature and pressure of properties on the vaporization behaviors for multi-component fuels. Then, utilizing the non-ideal approach to accurately predict the sensitive properties varied with pressure, and applying the simplified ideal approach to estimate the insensitive properties efficiently.

The primary aim of this study is to construct an accurate and efficient analogical multi-component (AMC) model to describe the vaporization behaviors of diesel droplets. To develop the AMC model, the influence of properties varied with components on the prediction accuracy of multi-component vaporization models need to be adequately understood. In order to better evaluate the performance of the AMC model, a discrete multi-component (DMC) model and a sequential multi-component (SMC) model, in fact, an enhanced single component model, were carried out. The outline of this paper is as follows. First, the proposed AMC and SMC, as well as the DMC models were briefly described. Then, the vaporization models were extensively validated by experimental measurements for multi-component diesel droplets. Finally, the computational accuracy and efficiency of the DMC, AMC, and SMC models were evaluated, and the vaporization characteristics of diesel droplets in the AMC model were discussed. The influence of the properties varied with component was analyzed in Appendix A-C. All the models were realized using an in-house code of Fortran 90.