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# Development of an improved hybrid multi-component vaporization model for realistic multi-component fuels

Ping Yi, Wuqiang Long, Ming Jia *, Liyan Feng, Jiangping Tian

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

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ABSTRACT

An improved hybrid multi-component (HMC) vaporization model was developed and applied to predict the vaporization characteristics of a realistic multi-component fuel droplet under various operating conditions in this study. Firstly, the realistic multi-component fuel is modeled as a mixture with a finite number of discrete hydrocarbon classes, and each hydrocarbon class is presented by a probability density function (PDF). Then, an HMC model was constructed based on the recent progress including an improved multi-diffusion sub-model, a corrected formulation for the calculation of Stefan flow velocity, and the temporal variation of thermal physical properties of fuels with temperature and compositions. The predictions of the improved HMC model were validated with the experimental data from literatures for the vaporization of realistic multi-component fuels and satisfactory agreements between the predictions and measurements are achieved. Finally, extensive comparisons of the hybrid multi-component (HMC), continuous multi-component (CMC), and discrete multi-component (DMC) models in the aspects of computational accuracy and efficiency were performed. It is found that the CMC model shows the highest computational efficiency and the lowest accuracy. The DMC model with a large amount of fuel components has the highest accuracy but the lowest efficiency. The HMC model not only could improve the computational efficiency compared with the full DMC model considering all fuel components, but also illustrates significantly better accuracy than the CMC model under the conditions tested in this study.



## 1. Introduction

Droplet vaporization plays an important role in internal combustion engine. For a more realistic description of the vaporization process of petroleum fuel droplet, the importance of development of multi-component vaporization model has been widely recognized recently [1–5]. The multi-component vaporization models are mainly classified into two types, i.e., continuous multi-component (CMC) model [6–8] and discrete multi-component (DMC) model [1,2,9].

In the CMC model, the fuel composition is described by a continuous probability density function (PDF) with appropriate parameters, such as molecular weight [10]. The CMC model shows significant advantages in terms of computational efficiency over DMC model. However, the computational accuracy of the CMC model with only a single distribution is insufficient, and the CMC model cannot be coupled with the multi-component detailed chemistry [1,11]. Moreover, the vaporization characteristics of the components with the same molecular weight in different hydrocarbon classes also cannot be reproduced by the CMC model.

In the DMC model, the realistic multi-component fuel is modeled as several discrete pseudo-components, and the physical properties of every pseudo-component are provided by the fuel libraries [12]. The DMC model can efficiently track the vaporization process of each discrete pseudo-component, and can be integrated with the reaction kinetics of the corresponding component [13]. Because it is difficult to consider all the individual components in gasoline and diesel fuels in the DMC model, and only several representative components are taken into account in most DMC models [1,14,15]. In this study, we consider the DMC model with all or most of the fuel components as full DMC model, and that with a small number of representative components as reduced DMC model. The light-end components (molecular weight is small) vaporize faster than the heavy-end components (molecular weight is large) during the vaporization process, so the selection of the components significantly affects the predictions of the DMC model [16].

* Corresponding author. Address: School of Energy and Power Engineering, Dalian University of technology, Dalian 116024, PR China. Tel./fax: +86 411 84706302.
*E-mail address:* jiaming@dlut.edu.cn (M. Jia).

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**Nomenclature**

| | |
|---|---|
| $a,b$ | boiling temperature constant |
| $A,B$ | function of temperature |
| $A_T$ | the averaged parameter |
| $C_p^g$ | specific heat capacity at constant pressure |
| $C_v^l$ | specific heat capacity at constant volume |
| $D_{i,j,1}^g$ | diffusion coefficient of species $i$ |
| $h$ | specific enthalpy |
| $f(I)$ | probability density function |
| $Gr$ | Grashof number |
| $I$ | molecular weight |
| $L$ | vaporization latent heat |
| $\dot{m}_{i,j,1}$ | mass vaporization rate |
| $Nu$ | Nusselt number |
| $P$ | ambient pressure |
| $P^{sat}$ | saturated vapor pressure |
| $P_{atm}$ | reference pressure |
| $Pr$ | Prandtl number |
| $q$ | heat flux vector |
| $Q_{conduction}$ | conduction heat flux |
| $Q_{enthalpy}$ | enthalpy diffusion |
| $Q_{gas}$ | total heat flux from gas mixture |
| $Q_{liquid}$ | heat flux absorbed by liquid |
| $R$ | droplet radius |
| $\overline{R}$ | gas constant |
| $Re$ | Reynolds number |
| $Sh_i$ | Sherwood number |
| $s_g$ | entropy constant |
| $T$ | gas mixture temperature |
| $T^b$ | boiling temperature |
| $T^d$ | droplet temperature |
| $T^f$ | reference temperature |
| $T^s$ | droplet surface temperature |
| $u$ | gas mixture velocity |
| $u^c$ | corrected velocity |
| $v$ | diffusion velocity |
| $x$ | mole fraction |
| $y$ | mass fraction |

*Greek symbols*

| | |
|---|---|
| $\alpha,\beta,\gamma$ | parameters for distribution function |
| $\Gamma(\alpha)$ | Gamma function |
| $\theta$ | mean molecular weight |
| $\psi$ | second moment of distribution |
| $\lambda^g$ | thermal conduction coefficient |
| $\sigma^2$ | distribution variance |
| $\rho$ | density |
| $\gamma_{i,j,1}$ | activity coefficient |

*Subscripts*

| | |
|---|---|
| $d$ | droplet |
| $i$ | spices |
| $k$ | discrete group |
| $j$ | hydrocarbon class |
| $s$ | droplet surface |

*Superscripts*

| | |
|---|---|
| $b$ | boiling temperature |
| $g$ | gas |
| $l$ | liquid |
| $sat$ | saturated |

It is worth noting that, for realistic multi-component fuels, the CMC model with a single distribution function cannot satisfactorily reproduce their compositions and physical properties. However, the DMC model with a large number of pseudo-components or all fuel components needs too long computational time to be implemented into computational fluid dynamics (CFD) simulation. Therefore, further improvement of the computational accuracy and efficiency of the vaporization model attracts increasing attentions [15,17].

Recently, a novel hybrid multi-component (HMC) model has been introduced [18–20], which combines the fundamental characteristics of the CMC and DMC models. In the HMC model, the multi-component fuels are modeled as several discrete classes, and each of which is described by a separate distribution function. Zhang and Kong [18,19] used the HMC model to describe the vaporization process of petroleum-biofuel droplets, and Yang et al. [20] (referred to DCMC model in Ref. [20]) applied the HMC model to simulate the vaporization of the droplet of realistic multi-component fuel. Compared with the DMC model, which contains a large amount of components as those in the realistic multi-component fuel, the HMC model significantly improves the computational accuracy. Moreover, the HMC model shows much higher computational accuracy relatively to the CMC model with a single distribution.

It is worth noting that, in the previous HMC model [18–20], the diffusion coefficients are assumed to be the same for all the hydrocarbon classes, and this simplification could result in increased error for the prediction of enthalpy diffusion of multi-components [21]. Therefore, it is necessary to consider the multi-components diffusion coefficients in the HMC model. Furthermore, the HMC model is still at the preliminary research stage, and the experimental verification has not been performed yet. Also, the performance of the HMC model compared with the DMC and CMC models in the aspects of computational accuracy and efficiency has not been well understood. Therefore, it is necessary to further evaluate and improve the HMC model, and find a compromised strategy for the multi-component vaporization model in order to simultaneously satisfy the requirement of the computational accuracy and efficiency for CFD simulation.

In this paper, an improved HMC vaporization model was developed to model the droplet vaporization process of realistic multi-component fuels. Firstly, the improved HMC model was briefly described. Then, the predictions of the improved HMC model were compared with the experimental results for the vaporization of realistic multi-component fuels. Finally, from the view of computational accuracy and efficiency, the HMC, CMC, and DMC models were evaluated, and the vaporization characteristics of different hydrocarbon classes in the HMC model were discussed.

## 2. Theoretical formulation

The physical model used in this study considers a spherical liquid droplet with multi-compositions in a nitrogen environment. As shown in Fig. 1, two major groups are divided in the computational model, i.e., fuel group ($C_mH_n$) and nitrogen group ($N_2$). The fuel group considers several discrete hydrocarbon classes according to those in the realistic multi-component fuels. Each hydrocarbon class, which is composed with an infinite number of species, is represented by a PDF distribution as that used in the CMC model. The computational domain is divided into four partitions (see Fig. 2), including droplet interior, liquid surface layer, gas surface