



The impacts of the activity coefficient on heating and evaporation of ethanol/gasoline fuel blends

Nawar Al-Esawi^a, Mansour Al Qubeissi^{a,b,*}, Sergei S. Sazhin^c, Reece Whitaker^b

^a Institute for Future Transport and Cities, Coventry University, Coventry CV1 5FB, United Kingdom

^b School of Mechanical, Aerospace and Automotive Engineering, Faculty of Engineering, Environment and Computing, Coventry University, Coventry CV1 2JH, United Kingdom

^c Advanced Engineering Centre, School of Computing, Engineering, and Mathematics, University of Brighton, Brighton BN2 4GJ, United Kingdom

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ABSTRACT

The evolutions of droplet radii and temperatures for ethanol and gasoline fuels and their blends are investigated using a modified version of the Discrete Component (DC) model, taking into account the effect of the activity coefficient (AC). The universal quasi-chemical functional-group AC (UNIFAC) model is used to predict the ACs of the blended ethanol and gasoline fuels approximated by 21 components. In contrast to previous studies, it is shown that droplet lifetimes predicted for pure gasoline are not always shorter than those predicted for ethanol/gasoline blends. They depend on the total vapour pressure of the mixture. It is shown that the original DC model predicts ethanol/gasoline fuel droplet lifetimes with errors up to 5.7% compared to those predicted using the same model but with the ACs obtained from the UNIFAC model.

1. Introduction

Heating and evaporation of droplets are important processes in numerous applications, including those in internal combustion engines [1,2], spray coating [3], fire suppression [4], the pharmaceutical industry [5], and agriculture [6,7]. This has stimulated intensive research to develop robust models for the description of these processes [1,8–10].

Our analysis is focused primarily on ethanol/gasoline fuel blend droplets, the interest in which has been mainly stimulated by the depletion of fossil fuels and environmental concerns. The heating and evaporation of these blends have been investigated numerically and experimentally [11–14]. In these studies, however, gasoline has been approximated by isooctane or a mixture of isooctane/n-heptane, whilst the commercial gasoline fuels consist of tens of hydrocarbons [15]. The effects of fuel compositions, transient diffusion of species, temperature gradient, and recirculation inside moving droplets on their heating and evaporation have been commonly described using the Discrete Component (DC) model [9,16], and the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model [8]. These models have been validated against experimental data [17–19].

The DC model was used previously for the analysis of blended fuel droplet heating and evaporation, including blends of diesel/biodiesel and ethanol/gasoline fuels [17,20–24]. In these studies, however,

Raoult's law was assumed to be valid (the activity coefficient (AC) was assumed equal to one). Unlike fossil fuels, ethanol and biodiesel fuels are polar liquids. Therefore, Raoult's law may not be suitable for predicting the vapour pressures of these fuel blends [25]. To address this issue, in our analysis we took into account the contributions of non-unity ACs. In some studies (e.g. [26]), the Wilson equation was used for the predictions of ACs. The Wilson equation is a simple approach, but limited to binary components. In the general case, the universal quasi-chemical functional-group AC (UNIFAC) model is believed to be the most suitable for prediction of the multi-component ACs [11,27].

In [28], the UNIFAC model was used to predict the ACs of 20 components in gasoline FACE C and 98 components in diesel fuel. This approach, however, was based on the initial molar fractions of components and droplet surface temperatures. In the current analysis, we investigate the impact of transient ACs on the evolutions of blended ethanol/gasoline fuel droplet temperatures and radii. The transient droplet surface temperatures and diffusion of 21 components are taken into account using the UNIFAC model. The governing equations and main features of the DC model used in our analysis are summarised in [8,29], and will not be discussed in this paper. The main features of the model and the implementation of UNIFAC equations into relevant equations of the DC model are described in Section 2. The results predicted by the modified DC model, using the corrected ACs, are presented and discussed in Section 3. The main results are summarised in Section 4.

* Corresponding author at: Institute for Future Transport and Cities, Coventry University, Coventry CV1 5FB, United Kingdom.

E-mail address: ac1028@coventry.ac.uk (M. Al Qubeissi).

2. The model

The DC model used in our analysis is based on the analytical solutions to the heat transfer and species diffusion equations inside droplets [9]. The effects of recirculation on species diffusion and heat conduction inside droplets are taken into account, using the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model [30]. The evaporation rate of a droplet is described by the following equation:

$$\dot{m}_d = -2\pi R_d D_v \rho_{\text{total}} B_M \text{Sh}_{\text{iso}}, \quad (1)$$

where D_v is the binary diffusion coefficient of vapour in gas (air), $\rho_{\text{total}} = \rho_g + \rho_v$ is the total density of the mixture of vapour and ambient gas (assumed not to depend on the distance from the droplet surface), Sh_{iso} is the Sherwood number for isolated droplets (taking into account the effects of droplet motion and evaporation), $B_M = \frac{Y_{\text{vis}} - Y_{\infty}}{1 - Y_{\text{vis}}}$ is the Spalding mass transfer number, and Y_{vis} and Y_{∞} are vapour mass fractions in the vicinity of the droplet surface and in the far-field, respectively, $Y_{\text{vis}} = \sum_i Y_{\text{vis}i}$ and $Y_{\text{vis}i}$ are the mass fractions of individual species i , calculated from the vapour molar fractions at the droplet surface ($X_{\text{vis}i}$) [16]:

$$X_{\text{vis}i} = \gamma_i \frac{X_{\text{lis}} p_{\text{vis}i}^*}{p}, \quad (2)$$

where p is the total (ambient) pressure, X_{lis} is the liquid molar fraction of the i^{th} species at the surface of the droplet, γ_i is the AC of the i^{th} species, and $p_{\text{vis}i}^*$ is the saturated pressure of the i^{th} species in the absence of other species.

In contrast to [10,17,20,24,31–33], where Raoult's law is assumed to be valid ($\gamma_i = 1$), our study accounts for the values of ACs taking into consideration the effect of corrected partial pressures of vapour components. The UNIFAC model is used for the estimation of the ACs of 21 components of ethanol/gasoline fuel blends. This model includes two terms: the combinatorial term (C) and residual term (R), taking into account the contribution of the excess entropy and the effect of the excess enthalpy, respectively. The excess entropy is inferred from various shapes and sizes of molecules or functional groups of atoms (hereafter referred to as groups, see Appendix A), while the excess enthalpy is inferred from interactions between molecules or groups [27,34]. The UNIFAC equation for the AC of component i in a multi-component mixture is presented as [35]:

$$\ln \gamma_i = \ln \gamma_i^{\text{C}} + \ln \gamma_i^{\text{R}}, \quad (3)$$

where $\ln \gamma_i^{\text{C}} = \ln \frac{\Phi_i}{X_i} + \frac{z}{2} q_i \ln \frac{\theta_i}{\Phi_i} + l_i - \frac{\Phi_i}{X_i} \sum_j X_j l_j$ is the combinatorial part, $\ln \gamma_i^{\text{R}} = \sum_k v_k^i (\ln \Gamma_k - \ln \Gamma_k^i)$ is the residual part, $l_i = \frac{z}{2} (r_i - q_i) - (r_i - 1)Z$, $Z = 10$, $\theta_i = \frac{q_i X_i}{\sum_j q_j X_j}$ is the area fraction of each molecule in the mixture, $\Phi_i = \frac{r_i X_i}{\sum_j r_j X_j}$ is the segment (volume) fraction of each molecule, $r_i = \sum_k v_k^i R_k$ is the volume parameter, $q_i = \sum_k v_k^i Q_k$ is the surface parameter, $\ln \Gamma_k = Q_k \left[1 - \ln \left(\sum_m \theta_m \psi_{km} \right) - \sum_m \frac{\theta_m \psi_{km}}{\sum_n \theta_n \psi_{nm}} \right]$, $\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n}$ is the area fraction of group m (see Appendix A), X_i is the molar fraction of liquid component i (the same as X_{lis} in Eq. (2)), X_m is the molar fraction of group m , and R_k and Q_k are the van der Waals volumes and surface areas for each group, respectively [34,35]. R_k is the volume occupied by each group in the molecule, while Q_k is the surface area occupied by each group in the molecule. Both R_k and Q_k are functions of bond distances, bond angles, contact distances, and shapes that are characteristic of the group [36]. The values of R_k and Q_k are presented in Table 4, Appendix A. v_k^i is the number of groups in molecule i . Γ_k is the residual AC of group k in the mixture and Γ_k^i is the residual AC of group k in a reference solution containing only molecules of type i (for example Γ_k^i for the CH_2OH group in ethanol refers to a solution containing 50% CH_2OH and 50% CH_3 , while CH_2OH in 1-pentanol refers to a solution of 20% CH_2OH , 60% CH_2 , and 20% CH_3). In other words, Γ_k^i deals with each group in each molecule, while Γ_k deals with each group in the

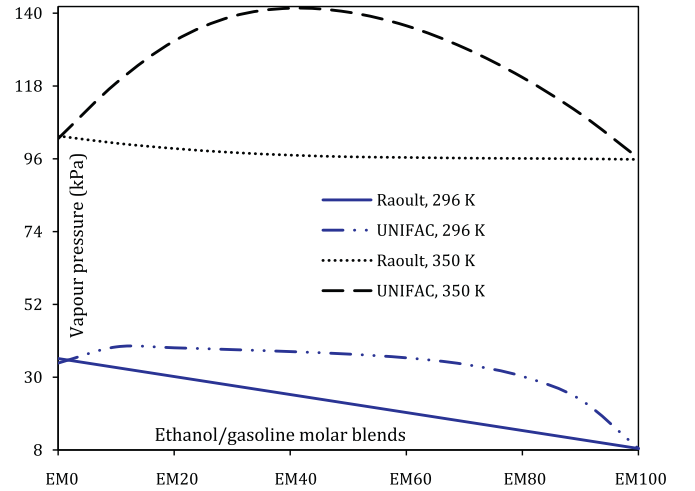


Fig. 1. Total vapour pressure of various ethanol/gasoline molar blends (EM0–EM100), predicted by Raoult's law and the UNIFAC model at $T = 296\text{K}$ and 350K .

mixture. $\psi_{mn} = e^{-\left(\frac{a_{mn}}{T}\right)}$ is the interaction and temperature dependent coefficient, a_{mn} is the group-interaction parameter between groups m and n (see Table 5, Appendix A) [35], m and n refer to the group in the mixture (in the case of Γ_k) or in the molecule (in the case of Γ_k^i). T is the interface temperature.

The liquid properties are calculated at the average temperature inside droplets, while the gas properties are calculated at the reference temperature $T_r = \frac{2}{3}T_s + \frac{1}{3}T_g$, where T_s and T_g are the droplet surface and ambient gas temperatures, respectively. Enthalpy of evaporation and saturated vapour pressure are estimated at T_s .

3. Results

The total vapour pressures versus molar fractions of ethanol/gasoline in the liquid phase (indicated as EMX, where X is the percentage of ethanol in the mixture) at 296 K and 350 K are presented in Fig. 1. In this figure, a comparison between the two approaches, Raoult's and UNIFAC, is shown. In Raoult's law, the AC is equal to unity, while in the UNIFAC model, the values of multi-component ACs are used.

As can be seen from this figure, the multi-component ACs have significant impact on the predictions of the total vapour pressure of ethanol/gasoline blends. For low ethanol molar fractions, breaks in the hydrogen bonds lead to a reduction in the inter-molecular forces [14]. This leads to an increase in the total vapour pressure. For high ethanol molar fractions, however, this pressure decreases as the contribution of the hydrogen bonds becomes important [14]. These predictions agree with those inferred from the experimental results presented in [37–39] (see Appendix B).

The heating and evaporation of blended ethanol/gasoline fuel droplets was investigated using the same operating conditions as in [17,32] but taking into account the impacts of non-unity ACs. The initial droplet radius was taken equal to $R_{do} = 12\ \mu\text{m}$, and its constant velocity in still air and initial temperature were assumed equal to $U_d = 24\ \text{m/s}$ and $T_{do} = 296\ \text{K}$, respectively. The ambient air pressure and temperature were assumed constant and equal to $p_g = 9\ \text{bar}$ and $T_g = 545\ \text{K}$, respectively.

The evolutions of droplet surface temperatures T_s and radii R_d versus time for various initial ethanol molar fractions (EM85, EM50, EM20 and EM5) are shown in Fig. 2. The mixtures EM85, EM50, EM20 and EM5 are approximately equivalent to the volume fractions 70% ethanol/30% gasoline, 29% ethanol/71% gasoline, 9% ethanol/91% gasoline, and 2% ethanol/98% gasoline, respectively. In this figure, the results predicted by four models are compared. The first one (labelled 'Ethanol/isooctane') is based on the transient UNIFAC model to predict

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