



Different spray droplet evaporation models for non-ideal multi-component fuels with experimental validation



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ABSTRACT

Herein three heat and mass transfer models were considered: the well-mixed (WM) model, the frozen evaporation (FZ) model and the diffusion controlled (DC) model for multi-component droplet evaporation were compared and validated against experimental data. The test fuels were mixtures of n-decane (a surrogate fuel for kerosene) and alcohol (ethanol or butanol) with differing volumetric ratios. Since the test fuels are non-ideal solutions, the activity coefficient of each fuel component was calculated by using the UNIFAC method and was incorporated with the heat and mass transfer models to account for the non-linearity effect on fuel evaporation process. Single-camera and PIV (Particle image velocimetry) measurements yielded the velocity distributions of fuel droplets at two cross-sections of the spray cone with different axial distances. The Sauter Mean Diameter (SMD) of spray droplets were measured by a LSA-III Malvern particle size analyzer. For butanol–decane blends, all the three different models can predict the evaporation accurately with little variation. Whilst, prediction of evaporation for ethanol–decane blends suffers much more noticeable variation among the models because of the relatively higher saturation vapor pressure of ethanol. A great deviation between the predicted droplet size and the measured SMD was observed for E10 (10% ethanol by volume) because the activity coefficient of ethanol for E10, and thus the evaporation rate, is more susceptible to the variation of the ethanol mole fraction. The well mixed model can be considered suitable for predicting slow evaporation processes with low injection pressures.

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1. Introduction

The fuel droplet evaporation process is critical in the combustion efficiency and the formation of emissions. A number of researchers [1–3] have considered one species liquid in stagnant environment, but in practice fuels are normally multi-component solutions [4,5]. The multi-component droplet evaporation has been studied theoretically and several models have been proposed [6–10].

The previous models can be divided into three categories: well mixed (WM) model, which indicates that when the external environment changes, the temperature distribution and the concentration distributions can be uniform instantaneously in the droplet; next is the frozen evaporation (FZ) model, which indicates that at any time of the evaporation, the temperature and the composition of the droplet is equal to the initial values; the final is the diffusion controlled (DC) model, in which the temperature and the component concentration vary temporally and spatially in the droplet [11–15].

However, few models have taken into consideration the effect of the activity coefficient of each component on the evaporation process. Some researchers have suggested the activity coefficient, but they assumed it as unity [14,16]. Thus, the mixtures were regarded as ideal solution which is consistent with Raoult's Law. In typical mixtures, Raoult's Law provides no more than an approximation: only when the components in the liquid mixture are similar, for instances a mixture of n-octane and iso-octane, can we assume that the activity coefficient is effectively unity for all components at all compositions [17]. For non-ideal multi-component mixtures, the activity coefficients of individual components can differ considerably from unity, and hence have a critical role in the calculation of vapor–liquid equilibria which governs the evaporation process.

There are several methods to calculate the activity coefficients for non-ideal solutions. For many moderately non-ideal binary mixtures, the more established methods (such as Margules, van Laar) are mathematically easier to utilize than the newer ones (Wilson, NRTL, UNIFAC). The Margules equation is applicable only to simple mixtures where the components are similar in chemical nature and in molecular size. For strongly non-ideal binary

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mixtures, such as solutions of alcohols with hydrocarbons, the equation of Wilson is most likely the most useful because it is mathematically simpler than the Non Random Two Liquid (NRTL) and Universal Quasi Chemical Functional Group Activity Coefficients (UNIFAC) equations. Previous research [11] used the Wilson method to calculate the activity coefficient for modeling fuel evaporation. However, experimental vapor–liquid equilibrium data are needed prior to using the Wilson method. Furthermore, it is not accurate and practical to extend binary data to multicomponent mixtures with the Wilson method. Therefore, the UNIFAC, a group contribution method [18], was adopted in this study to obtain the activity coefficients of individual components without any experimental vapor–liquid equilibrium (VLE) or liquid–liquid equilibrium (LLE) data.

Three commonly used heat and mass transfer models for multi-component fuel evaporations, namely, the WM, FZ, DC models have been extensively investigated [19]. The objective of this paper is to incorporate the non-ideality effects (via the activity coefficient determination) into the existing models. The relative velocity between the droplet and the surrounding air may enhance the evaporation significantly, therefore, it is desirable to obtain the droplet velocity as accurately as possible. In order to validate the models in a more accurate way, the droplet velocities (as the model inputs) were experimentally obtained using particle image velocimetry (PIV) rather than a value calculated according to a theory [20] or a constant value assumed according to an empirical set of equations [11,14,15,19,21].

2. The theory of the multi-component fuel evaporation models

2.1. Activity coefficient determination

At a specific temperature and pressure, the fuel vapor pressure of each component in the mixture is strongly related to the enthalpy of evaporation and the activity coefficient of each component. The fundamental equation governing multi-component vapor–liquid equilibrium is the modified Raoult’s law:

$$y_i p = \gamma_i x_i p_{vpi} \quad (1)$$

where y_i is mole fraction of the i th species in the vapor, p is total pressure, and γ_i is the activity coefficient of the i th species, p_{vpi} is the saturation vapor pressure of the i th species, x_i is the mole fraction of the i th species in the liquid. To calculate the activity coefficient accurately, the UNIFAC method was adopted.

According to the UNIFAC method, the molecular activity coefficient consisted of two parts: the combinatorial component (γ_i^c) and the residual component (γ_i^R). In a multi-component mixture [22], the UNIFAC equation for the activity coefficient of component i can be given as:

$$\ln \gamma_i = \ln \gamma_i^c + \ln \gamma_i^R \quad (2)$$

The combinatorial component provided the contribution to activity coefficients because of differences in the sizes and shapes of the molecules, and the residual component provided the contribution because of molecular interactions. The combinatorial part is estimated using the following equations:

$$\ln \gamma_i^c = \ln \left(\frac{\varphi_i}{x_i} \right) + \frac{Z}{2} q_i \ln \left(\frac{\theta_i}{\varphi_i} \right) + L_i - \frac{\varphi_i}{x_i} \sum_j x_j L_j \quad (3)$$

$$\varphi_i = \frac{r_i \cdot x_i}{\sum_j r_j \cdot x_j}, \quad \theta_i = \frac{q_i \cdot x_i}{\sum_j q_j \cdot x_j} \quad (4)$$

$$L_i = \frac{Z}{2} (\gamma_i - q_i) - (\gamma_i - 1), \quad Z = 10 \quad (5)$$

where x_i represents the mole fraction of component i , and the summations in Eqs. (3) and (5) are over all components, including component i ; the definitions of other parameters such as φ_i , r_i , θ_i , q_i can be found elsewhere [17]. Parameters r_i and q_i are calculated as the sum of the group volume and area parameters R_k and Q_k , which are:

$$\gamma_i = \sum_{k=1} v_k^{(i)} R_k \quad (6)$$

$$q_i = \sum_{k=1} v_k^{(i)} Q_k \quad (7)$$

where $v_k^{(i)}$, always an integer, is the number of groups of type k in molecule i . Group parameters R_k and Q_k are obtained from the Van-der Waals group volume and surface areas V_{wk} and A_{wk} , given by Bondi [23]

$$R_k = \frac{V_{wk}}{15.17} \quad \text{and} \quad Q_k = \frac{A_{wk}}{2.5 \times 10^9} \quad (8)$$

The residual part of the activity coefficient, which depends on group areas and group interaction, is replaced by the solution-of-groups concept as shown below:

$$\ln \gamma_i^R = \sum_k v_k^{(i)} \left[\ln \Gamma_k - \ln \Gamma_k^{(i)} \right] \quad (9)$$

where Γ_k is the group residual activity coefficient and $\Gamma_k^{(i)}$ represents the residual activity coefficient of group k in a reference solution containing only molecules of type i .

The group activity coefficient Γ_k can be calculated as follows:

$$\ln \Gamma_k = Q_k \left[1 - \ln \left(\sum_m \theta_m \psi_{mk} \right) - \sum_m \frac{\theta_m \psi_{km}}{\sum_{l=1}^n \theta_l \psi_{lm}} \right] \quad (10)$$

This equation also holds for calculating $\ln \Gamma_k^{(i)}$. The value of θ_m is the area fraction of group m , and the sums are over all different groups. The value of θ_m is calculated as follows

$$\theta_m = \frac{Q_m X_m}{\sum_n Q_n X_n} \quad (11)$$

where X_m is the mole fraction of group m in the mixture. The group-interaction parameter ψ_{mn} is given by

$$\psi_{mn} = \exp \left(- \frac{U_{mn} - U_{nm}}{RT} \right) = \exp \left(- \frac{a_{mn}}{T} \right) \quad (12)$$

where U_{mn} is a measure of the energy of interaction between groups m and n . Parameters a_{mn} and a_{nm} are obtained from a database using a wide range of experimental results and can be referred elsewhere [24]. Numerical values of parameters R_k , Q_k and a_{mn} are provided elsewhere [13,23–25].

2.2. Heat and mass transfer models of fuel droplets

For the droplets evaporation at the atmosphere, the initial droplet temperature and the surrounding air temperature are all 303 k which is higher than the wet bulb temperature (the temperature a parcel of air would reduce to if it were cooled by the fuel evaporating until the air was saturated with the fuel vapor). Hence the droplets will experience two phases of evaporation: firstly the droplets evaporate as the temperature falls to the wet bulb temperature, and secondly the droplets evaporate with the constant wet bulb temperature. The cooling of the multi-component droplets is governed by the following transient heat conduction equation:

$$\frac{\partial T}{\partial t} = a \left(\frac{\partial^2 T}{\partial r^2} + \frac{2}{r} \frac{\partial T}{\partial r} \right) \quad \text{and} \quad a = \frac{\lambda_L}{\rho_L c_{pL}} \quad (13)$$

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