

A Multi-Distribution Functions Droplet Evaporation Model using Continuous Thermodynamics

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ABSTRACT

A finite diffusion method is presented in this paper to model droplet evaporation for complex liquid mixture composed of different homogeneous groups. Multiple components fuel mixture is represented by separate distribution functions to describe the composition of each homogeneous group in the mixture. Only a few parameters are required to describe the mixture. Quasi-steady assumption is applied in the determination of evaporation rates and heat flux to the droplet, and the effects of surface regression, finite diffusion and preferential vaporization of the mixture are included in the liquid phase equations using an effective properties approach. The proposed model was validated by comparing against experimental measurements for single, isolated droplets of n-decane, kerosene, heptane-decane and diesel-butanol. The present model was applied to simulate the evaporation of isolated droplets with composition of typical diesel. Computations showed that the model captured the main distillation characteristics of commercial fuels reasonably well. The proposed model is capable in capturing the vaporization characteristics of complex liquid mixtures.

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INTRODUCTION

Commercial fuels are mixtures of hundreds of chemically different hydrocarbons with vastly different boiling points that could range from 340 K to over 700 K. Law [1] pointed out that liquid motion within the droplet, miscibility among the liquid components and relative volatilities of the components are the three controlling factors in the understanding of multi-component fuel behavior. The immensely different volatilities among the components imply significant different evaporation rates. Moreover, the liquid constituents can evaporate only if it reaches the surface. As more volatile species evaporates, less volatile constituents become dominating within the liquid phase. As a result, the species mass fractions and temperature are no longer uniform within the droplet. This process is known as preferential evaporation. In most numerical simulations, the fuel is usually represented by a single component, for example, tetradecane ($C_{14}H_{30}$) is usually used to represent

commercially available diesel. A major deficiency with this approach is that the influence of fuel composition is not accounted for, and, only the average evaporation behavior can be obtained. A possible solution to this is to use a set of fuel constituents to reproduce the distillation curve. An accurate representation of the fuel is essential for acquiring insightful information out of a simulation. The volatility of fuel maintains a dominant position on spray penetration and ignition is controlled by the most volatile species in the mixture [2, 3]. However, to represent each component in a commercial fuel, consists of hundreds of component, using a discrete representation is impractical. Not only every component requires a separate transport equation, the exact composition is in generally unknown.

As an alternative, continuous thermodynamics provides a more effective solution. The mixture is characterized by a probability distribution function (PDF) with respect to some characterizing variable(s), for examples, molecular weight or boiling points. Only a few parameters are required to describe

the mixture, namely, the mean and variance of the probability distribution function. This approach was first developed in chemical engineering and has been applied in a variety of calculations including vapor-liquid equilibrium, liquid-liquid equilibrium, flash boiling and characterization of hydrocarbon mass fraction. It was first used for investigating the vaporization of isolated droplets by Tamim and Hallett [4]. The gas phase transport equations were solved with fine grid spacing close to the droplet surface. But this is infeasible for multi-dimensional spray simulations, which involve thousands of droplet parcels and complex engine geometry. Hallett [5] presented a quasi-steady analytical solution for droplet vaporization and applied his model to computations of diesel and gasoline, which captured important features, such as the distillation curves of commercial fuels, quite well. This model was extended to fuel droplet vaporization in a high-pressure environment [6]. The method of continuous thermodynamics has been applied in multi-dimensional engine modeling for spray calculations [7,8,9,10,11]. These studies made important contributions to the application of continuous thermodynamics to internal combustion engine simulations. However, most of the previous studies [9,10,11,12,13,14,15,16,17,18] are based on the assumption of infinite diffusion in the liquid phase, so non-uniformity inside the droplet is not considered.

The evaporation of fuel in high pressure ambient has been investigated extensively in the literature [12,13,14,15,16], since fuel evaporates in high-pressure ambient in many engineering applications. Ghassemi et al. [13, 14] reported the evaporation of droplets behaved differently at elevated ambient pressure. The evaporation of a bi-component droplet occurs in three stages, which was unseen from a single-component droplet. Most of the component with lower boiling point evaporated first, then, a non-evaporative heat-up process, followed by the evaporation of the less volatile component. There were attempts in modeling high-pressure evaporation of fuel droplets using zero-dimensional models, for applications in multi-dimensional engine simulations. Zhu and Aggarwal [17] studied the effects of equations of state on droplet transient evaporation and concluded that the Peng-Robinson equation of state predicted the droplet evaporation accurately. Aggarwal and Mongia [18] developed a high-pressure evaporation model accounting for multi-component effect. The study concluded that elevating ambient pressure lengthened the heat up process, but variation in ambient pressure did not visibly affect the droplet lifetime. Tonini et al. [19] presented a spray calculation using the high-pressure vaporization model by Aggarwal and Mongia [18]. The authors concluded that zero-dimensional models would provide enough accuracy in engine simulations, considering the uncertainties from droplet breakup and collision, vapor-phase turbulence and droplet-turbulence interactions in such calculations. Wang and Lee [20] proposed a model using the continuous thermodynamics formulation in order to account for high-pressure effects. Gas solubility imposed significant effects on the droplet breakup as it altered surface tension.

Consequently, the predicted spray structure, fuel-vapor distribution and engine performance were considerably different than droplet evaporating at atmospheric ambient.

In this paper, a comprehensive model considering preferential vaporization of a complex fuel mixture using continuous thermodynamics without the infinite diffusion assumption in the liquid phase is presented. This approach uses only three equations to trace the mass transfer process: one for the mole fraction, one for the first moment and another one for the second moment of the probability distribution function used to represent the mixture. Therefore, it eliminated the need to trace the evolution of each component independently. The improvement in computational efficiency is embedded in the mathematical formulation. This could be a significant improvement in computational efficiency especially in cases of complicated mixtures. The model consists of a gas phase sub-model which determines evaporation rates and heat flux, and a liquid phase sub-model with finite diffusion.

GAS PHASE EQUATIONS

A fuel mixture is described by a continuous probability distribution function, $f(\omega)$, characterized by the molecular weight, ω , of each component. The fraction of a component is $y_F f(\omega_i) d\omega$, where y_F is the total molar fraction of fuel in gas phase, and in this study, $f(\omega)$ is a Γ -distribution function, which is often used to represent petroleum fractions [20],

$$f(\omega) = \frac{(\omega - \gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp\left(-\frac{\omega - \gamma}{\beta}\right), \quad (1)$$

where γ is the origin, α and β are parameters controlling the shape of the probability distribution function, with the mean molecular weight, $\theta_1 = \alpha\beta + \gamma$, and the variance, $\sigma^2 = \alpha\beta^2$. In

previous studies, using the second moment, $\theta_2 = \sigma^2 + \theta_1^2$, was found to be more convenient for calculations than using the variance [12]. Here, θ_j is the j^{th} moment of $f(\omega)$. The transport equations for energy and molar fuel fraction, y_F , can be obtained by integrating energy and species conservation equations over the probability distribution function and two additional transport equations for θ_1 and θ_2 are achieved by performing proper weightings over the equation for fuel fraction. The gas phase transport equations for droplet vaporization, using continuous fuel representation, were first completed by Tamim and Hallett [12].

The methodology is similar to previously studies within the frame work of continuous thermodynamics. The vapor-phase quasi-steady solutions are given by:

$$\dot{N}'' = \frac{Sh_i}{2} \frac{C_{vap} D_{0i}}{R} \ln(1 + B_j), \quad (2)$$

$$\dot{N}_{\psi_j}'' = \dot{N}'' \left[\Phi_{j,R} - \frac{\Phi_{j,R} - \Phi_{j,\infty}}{1 - (1 + B_j) \frac{D_{0j}}{D_{\psi_j}}} \right], \quad (3)$$

where $\dot{N}''$ is the total vapor flux, and $\dot{N}_{\psi_j}''$ is the flux for j^{th} moment; D_{ψ_j} and D_{0j} is the average diffusivity for fuel composition and j^{th} moment, respectively, and B_j is the transfer number given by,

$$B_j = \frac{y_{j, \text{surf}} - y_{j, \infty}}{\frac{\dot{N}_{\psi_j}''}{\dot{N}''} - y_{j, \text{surf}}}. \quad (4)$$

Note that the Sherwood number is evaluated using fuel fraction, since the diffusivities for composition and the moments are almost the same. The heat flux to the droplet, $\dot{q}''$, is given by,

$$\dot{q}'' = \dot{N}'' \left[\frac{C_p (T_{\infty} - T_R)}{\exp\left(\frac{2 \dot{N}'' C_p R}{k_{\text{vap}} Nu - 1}\right)} - \Delta H_{fg} \right], \quad (5)$$

where C_p , ΔH_{fg} , k_{vap} and Nu are the vapor phase specific heat capacity, latent heat for vaporization, thermal conductivity and Nusselt number, respectively.

LIQUID PHASE EQUATIONS

The transient behavior of the liquid phase significantly affects the evaporation of a spray and thus, the vapor distribution. In the present study, an effort is made to properly model the non-uniformity of liquid phase due to finite diffusion vaporization rather than using the infinite diffusion model as in the study by Tamim and Hallett [4]. The transport equations for the liquid phase are obtained with the same approach as used in the gas phase. The complete liquid phase equations are too complex to be solved analytically. Previous studies on the liquid phase during droplet vaporization have provided a lot of knowledge and inspiration on the simplifications to the problem while retaining reasonable accuracy. Internal circulation enhances diffusion in the liquid phase and this effect can be accounted for by an effective diffusivity and conductivity [21, 22]. In addition, assuming that in a short time interval, molar concentration and specific heat are constant, and that the flow is symmetric since the effects of internal vortices are included in the effective properties [23], the liquid phase equations can then be simplified and written as:

$$\frac{\partial C_{liq} \vec{\Phi}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 C_{liq} D_{\phi} \frac{\partial \vec{\Phi}}{\partial r} \right), \quad (6)$$

where the subscript *liq* represents liquid phase, $\vec{\Phi}$ is a vector of $\{\Phi_j\}_{j=1}^N$. Note that the diffusivities in equation (6) are multi-component diffusivities, which are in general given by,

$$D_{\phi} = B^{-1}, \quad (7)$$

for an ideal mixture. The elements of B are calculated from the binary diffusion coefficients and molar composition of the mixture as,

$$B_{ii} = \frac{y_i}{D_{iN}} + \sum_{\substack{k=1 \\ i \neq k}}^N \frac{y_i}{D_{ik}}, \quad B_{ij} = -y_i \left(\frac{1}{D_{ij}} - \frac{1}{D_{iN}} \right). \quad (8)$$

The boundary conditions for liquid phase are given by,

$$\left. \frac{\partial \vec{\Phi}}{\partial r} \right|_{r=0} = 0, \quad C_{liq} D_{\phi} \left. \frac{\partial \vec{\Phi}}{\partial r} \right|_{r=R} = \dot{N}'' \vec{\Phi} - \dot{N}_{\phi_j}'' = \vec{\Omega}_{\phi}. \quad (9)$$

The conductivity and diffusivities in the equations are all effective properties. Symmetry imposes the boundary conditions at the droplet center, and conservation conditions are applied at the droplet surface,

$$\left. \frac{\partial \vec{\Phi}}{\partial r} \right|_{r=0} = 0, \quad C_{liq} D_{\phi} \left. \frac{\partial \vec{\Phi}}{\partial r} \right|_{r=R} = N_{Y_f} \vec{\Phi} - N_{\phi} = \vec{\Omega}_{\phi}. \quad (10)$$

Equation (6) represents a system of coupled partial differential equations, for which an exact, analytical solution is in general unavailable as the diffusivity matrix, D_{ϕ} , strongly depends on mixture composition. The solution can be computationally intensive, even if efficient numerical techniques are employed. If C_{liq} and D_{ϕ} are assumed constant, as in Toor [24] and Stewart and Prober [25],

$$C_{liq} \frac{\partial \vec{\Phi}}{\partial t} = C_{liq} D_{\phi} \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \vec{\Phi}}{\partial r} \right), \quad (11)$$

the system of equations can then be linearized and decoupled by decomposing the diffusivity matrix using eigenvalue decomposition. It has been shown that eigenvalue decomposition always exists for the diffusivity matrix [26],

$$A = \Sigma^{-1} D_{\phi} \Sigma, \quad (12)$$

where A is the diagonal eigenvalue matrix, and Σ is the associated eigenvector matrix. Substitute equation (12) into equations (10) and (11) and multiply each of the equations by Σ^{-1} , yielding equations (13) and (14).