

RESEARCH PAPER

Comparative Analysis of a Single Fuel Droplet Evaporation

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Abstract

In this research, the results of comparative analysis of a single fuel droplet evaporation models are presented. Three well-known evaporation models including Spalding, Borman-Johnson and Abramzon-Sirignano models are analyzed using Computational Fluid Dynamic (CFD). The original Spalding model is extended to consider the effects of the Stefan flow, unsteady vaporization, and variable properties. The evaporation models are validated using already existing experimental data. Numerical results show that the Spalding model overestimates the temperature of the droplet surface in comparison with the other two models, although some modifications were made in the aforementioned model. Our final evaluation concludes that Abramzon-Sirignano model predictions are in good agreement with the experimental data. Therefore, in this paper, this model is used for the parametric study of the effects of droplet size, ambient temperature and pressure on the droplet lifetime and temperature. Results indicate that by increasing the droplet size, the lifetime of the droplets will increase and the steady-state droplet temperature is higher at higher ambient pressures and temperature.

Introduction

The process of vaporization is considered to be a challenging issue, due to the inclusion of both heat and mass transfer [1]. When a liquid is exposed to a hot gas, heat transfer occurs from the hot gas to droplets by means of conduction and convection, while the vapor is transferred by diffusion and convection. Vaporization of a droplet involves the heat, mass and momentum transfer between the gas and liquid phases, and their coupling at the droplet interface. Evaporation has a variety of applications such as spray combustion, spray drying, etc. In the past, the design of these systems was usually based on experience. with the high cost and non-optimal quality of the products. Nowadays Computational Fluid Dynamics (CFD) tool is applied to simulate spray and evaporation processes .Better understanding and modeling of complex spray flows depends significantly on the selected model for droplet vaporization analysis [2]. So many researchers have studied the evaporation of a single fuel droplet numerically and experimentally [2-7]. Spalding [8] proposed a model for quasi-steady vaporization rate of a single stationary droplet in an infinite, constant temperature and air

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(1)

velocity. After that, Spalding [8] modified the model to take into account the effects of forced convection. However, in the classical Spalding model, the effect of the Stefan model was ignored. Borman-Johnson [9] developed a model for unsteady vaporization of Fuel drops. Abramzon and Sirignano [2] developed an accurate model for droplet vaporization that considered the effects of variable properties, non-unitary Lewis number, and Stefan flow via film theory on heat and mass transfer between the droplet and the gas phase.

In the present research, the Spalding, Borman-Johnson, and Abramzon- Sirignano models are used to capture the evaporation process of the droplet using a homemade evaporation code. The Spalding model is modified to consider the effect of Stefan flow by correcting the Nusselt number. In this study, a single fuel droplet is injected into a gaseous environment. Fuel droplet and gaseous environment are considered n_decane and air, respectively. The interaction between droplet and gas is assumed to be one-way coupling, which means that the effects of droplet motion on the gas phase are ignored. So, the gas temperature, pressure, and velocity components are assumed to be constant. The results of these modeling are compared with the experimental measurements of Wong et al. [3] and the most compatible model with experimental data is determined.

Evaporation Models

In this section, three already mentioned evaporation models reviewed and some modifications were made to the Spalding model in order to increase its accuracy.

Modified Spalding Model

According to the classical Spalding droplet evaporation theory [10], the stationary vaporization rate of a single droplet in an infinite, constant temperature and constant velocity air environment is given by:

$$\dot{m} = 2\pi d\rho_m D_{diff} \ln(1 + B_M) \tag{1}$$

where d, ρ_m , D_{diff} and B_M are droplet diameter, mixture density, diffusion coefficient and Spalding mass transfer number, respectively. Eq. 1 is suitable for a single fuel droplet in a quiescent flow. Therefore, Eq. 1 must be corrected for the influence of forced convection. In the forced convection flow, researchers have proposed many correlations for estimating Nusselt and Sherwood number. The most widely used is the Ranz –Mrshall equation which is given as [11]:

$$Nu_0 = 2 + 0.552 \text{Re}^{1/2} \text{Pr}^{1/3}$$
(2)

$$Sh_0 = 2 + 0.552 \text{Re}^{1/2} \text{Sc}^{1/3}$$
(3)

where Re, Pr, and Sc are Reynolds, Prandtl, and Sherwood numbers, respectively. So, in this study the vaporization rate of a single droplet in forced convection flow is calculated by the following equation:

$$\dot{m} = \pi d\rho_m D_{diff} \mathrm{Sh}_0 \mathrm{ln}(1 + B_M) \tag{4}$$

where Sh_0 is the Sherwood number without considering Stefan flow effect. The Spalding mass transfer number, fuel vapor mass fraction and molar fuel vapor fraction at the droplet surface formulas are as follows:

$$B_M = \frac{y_{FS} - y_{F\infty}}{1 - y_{FS}} \tag{5}$$

$$x_{FS} = \frac{P_{FS}}{P} \tag{6}$$

$$y_{FS} = \frac{x_{FS} M W_l}{x_{FS} M W_l + (1 - x_{FS}) M W_g}$$
(7)

where x_{FS} , P, P_{FS} , y_{FS} and MW are fuel vapor molar fraction, total pressure, fuel vapor saturated pressure, fuel vapor mass fraction and molecular weight. The subscripts g and l refer to gas and liquid, respectively. Fuel vapor saturated pressure for n-decane is calculated by using the experimental correlation as follows [2]:

$$P_{FS} = \exp(11.495 - 5141/T_d) \tag{8}$$

In the classical Spalding model, the temperature of the droplet was assumed to be constant at wet bulb temperature and also thermodynamic properties were considered to be constant. But it was proved that variable temperature and thermodynamic properties have an important effect on the evaporation process [2]. So, in this research, in order to increase the accuracy of the model, thermodynamic properties are evaluated using Borman-Johnson method for taking into account the effect of droplet temperature variation on thermodynamic properties. The properties of liquid fuel are calculated at liquid temperature whereas the properties of fuel vapor are calculated by the average temperature that is defined as:

$$T_m = \frac{T_g + T_l}{2} \tag{9}$$

where T is the temperature. The subscripts g and l refer to gas and liquid, respectively. Average physical properties (such as viscosity, thermal conductivity and specific heat at constant pressure) of the mixture of fuel vapor and hot gas in the gas film are calculated as follows:

$$N_{mixture} = N_{gas} \times (1 - pratio) + N_{fuelvapor} \times pratio$$
(10)

in which *N* is a physical property and *pratio*, is the ratio of the partial pressure to the total pressure which is calculated from the following equation:

$$pratio = 0.5 \frac{PFV}{P} \tag{11}$$

where *PFV*, is partial fuel vapor pressure at droplet surface, for n-decane which is calculated by:

$$PFV = \exp(11.495 - 5141/T_d) \tag{12}$$

The convective flow of fuel vapor from the droplet surface into the gas phase is known as Stefan flow. Stefan flow results in the thermal and mass boundary layer to become thicker. In the classical Spalding model, the effect of the Stefan model was ignored. But in this paper the effect of this phenomenon is taken into account by correcting the Nusselt number as follows:

$$Nu = Nu_0(\frac{z}{e^z - 1})$$
(13)

In Eq. 13, $z/(e^z - 1)$ is an experimental coefficient which corrects the heat transfer coefficient, when the mass transfer is simultaneously taking place and z is defined by Bird et al. [12] as follows:

$$z = -\frac{C_{PV}(\frac{dm}{dt})}{\pi dk Nu}$$
(14)

A quasi-steady assumption was utilized in Spalding initial approach. Since then, it has been proved that the transient droplet heating phenomena have an important effect on the evaporation process [10]. So, in this work, the energy equation for determining the surface temperature of the droplet is defined as:

$$\frac{d(mC_PT)_d}{dt} = \pi dk \left(T_{gas} - T_d\right) \times \left(\frac{z}{e^z - 1}\right) \operatorname{Nu} + Q \frac{dm_d}{dt}$$
(15)

where C_P and k are droplet specific heat and thermal conductivity, respectively. In the classical model, Spalding proved that the droplet-squared diameter decreases linearly with the time that is known as d-square law. Its equation is shown below:

$$td^{2} = d_{0}^{2} - \frac{8\rho_{g}D_{diff}}{\rho_{l}}\ln(1+B_{M})$$
(16)

where d, ρ_g , ρ_l , D_{diff} , B_M and t are droplet diameter, gas density, liquid density, diffusion coefficient, Spalding mass transfer number and time, respectively. The subscript 0 refers to the initial condition.

Borman-Johnson Model

Calculations of liquid fuel, gas and fuel vapor/ air mixture properties in the gas film are considered to be the same as the Spalding model. But in this model droplet mass history is calculated by the following equation:

$$\frac{dm_d}{dt} = -\pi dD_{diff} P \times \ln\left(\frac{P - P_{\nu,\infty}}{P - PFV}\right) Sh/(RT_m)$$
(17)

where m_d and R are mass of droplet and gas constant, respectively. The equation for determining the surface temperature of the droplet is considered the same as the Spalding model (Eq. 15).

Abramzon and Sirignano Model

Abramzon and Sirignano [2] developed an accurate model for droplet vaporization. In the present model, the effects of variable properties, non-unitary Lewis number, and Stefan flow on heat and mass transfer between droplet and gas phase were considered. For considering the effect of Stefan flow, the so-called film theory was adopted. Diffusional and thermal correction factors of film thicknesses were used to consider the effect of the Stefan flow. Average physical properties of the fuel vapor/ air mixture in the gas film was calculated at some reference temperature and fuel vapor mass fraction as follows:

$$\bar{T} = T_{S} + A_{r}(T_{\infty} - T_{S})$$

$$\bar{y}_{F} = y_{FS} + A_{r}(y_{F\infty} - y_{FS})$$
(18)
(19)

where the value of A_r coefficient is set to be 1/3. After calculating mixture properties in the gas film, mole and mass fraction of fuel vapor at the droplet surface and Spalding mass transfer number were calculated like the Spalding model. Since Ranz-Marshall correlations overestimate Nusselt and Sherwood numbers (Eqs. 2 and 3) at low Reynolds number (Re \leq 10), the correlation suggested by Clift et al. [13] are used in the present study:

$$Nu_0 = 1 + (1 + \text{RePr})^{1/3} f(\text{Re})$$
(20)

$$Sh_0 = 1 + (1 + \text{ReSc})^{1/3} f(\text{Re})$$
(21)

Where f(Re) is calculated by:

$$f(\text{Re}) = \begin{cases} 1, & \text{Re} \le 10 \\ \text{Re}^{0.077}, & \text{Re} \ge 400 \end{cases}$$
(22)

Then the value of correction factor of the diffusional film thicknesses corrected Sherwood number, vaporization rate, correction factor of the thermal film thicknesses, corrected Nusselt number, non-dimensional parameter \emptyset and Spalding heat transfer number are defined as follow:

$$F(B_M) = (1 + B_M)^{0.7} \frac{\ln(1 + B_M)}{B_M}$$
(23)

$$Sh^* = 2 + (Sh_0 - 2)/F(B_M)$$
 (24)

$$\dot{m} = \pi d\rho_m D_{diff} Sh^* \ln(1 + B_M) \tag{25}$$

$$F(B_T) = (1 + B_T)^{0.7} \frac{\ln(1 + B_T)}{B_T}$$
(26)

$$Nu^* = 2 + (Nu_0 - 2)/F(B_T)$$
(27)

$$\phi = \left(\frac{C_{PF}}{\bar{C}_{Pg}}\right) \left(\frac{\mathrm{Sh}^*}{\mathrm{Nu}^*}\right) \frac{1}{\mathrm{Le}}$$
(28)

$$B_T = (1 + B_M)^{\emptyset} \tag{29}$$

where Sh^{*}, B_T and Nu^{*} are corrected Sherwood number, Spalding heat transfer number and corrected Nusselt number respectively. After determining the value of B_T , recalculations of the parameters B_M , $F(B_M)$, Sh^{*}, \dot{m} , $F(B_T)$, Nu^{*} and \emptyset are performed until the following condition is reached:

$$\left|B_T - B_T^{old}\right| < \varepsilon \tag{30}$$

In the above equation, ε is the desired accuracy of the B_T that in this work is set as 0.0001. Then, the heat penetrating into the liquid phase is calculated by the following equation:

$$Q_l = \dot{m} \left\{ \frac{\bar{C}_{PF}(T_g - T_S)}{B_T} - L(T_S) \right\}$$
(31)

After determining the value of Q_l , the new time step values of droplet diameter and temperature are obtained by solving the following equations:

$$\frac{dr_s}{dt} = -\frac{\dot{m}}{4\pi\rho_l r_s^2} \tag{32}$$

$$m_p C_p \frac{dT}{dt} = Q_l \tag{33}$$

Results and Discussions

The aim of this study is to provide a comparative analysis of a single fuel droplet evaporation models. A CFD code is developed in order to calculate the surface temperature, non-

dimensional radius, and vaporization rate using three different models consisting of Modified Spalding, Borman-Johnson and Abramzon- Sirignano models. These evaporation models are validated against experimental data which are gathered by Wong et al [3]. The fuel considered in this study is n_decane. Initial diameter and temperature of the n_decane droplet are 2000 (μ m) and 315 (K), respectively [3]. The n-decane droplet is exposed to the hot air stream of constant velocity, temperature and pressure which are fixed at 1m/s, 1500 (K) and 1 (atm) respectively [3]. When a droplet is exposed to a hot gas, its temperature starts to rise until it reaches to wet bulb temperature. At the wet-bulb temperature, all the energy reaching droplet are utilized to evaporate the droplet. According to experimental results, when the temperature of a droplet reaches the wet bulb temperature, it generally remains near the wet-bulb temperature without a significant increase. Therefore, evaporation of the droplet consists of two part, heat up period and steady-state period. Through the heat up period, the temperature of the droplet increases, while the vapor is produced until the drop reaches the steady-state temperature.

Fig. 1 shows the variation of the surface temperature of the n_decane droplet during its lifetime for three models of evaporation mentioned above. The results are compared with experimental data. The general trend of all curves in Fig. 1 depicts that during the early stages of droplet lifetime heat transfer from the ambient gas contributes to heating the droplet interior rather than vaporization and the droplet temperature increases until it reaches the wet-bulb temperature. The vapor is produced when the droplet reaches the wet-bulb temperature and after that, the droplet temperature will gradually increase. These two periods are obvious in Fig. 1. Also, results indicate that, in spite of the modifications made to the Spalding model, still this model overestimates the temperature of droplet surface in comparison with other two models and the predictions by the Abramzon-Sirignano model is more consistent with experimental results.



Fig. 1. variation of droplet surface temperature with respect to time

A little reduction in the non-dimensional droplet diameter and hence in Reynolds number was observed during the heat up period for all models. In the initial period of the droplet lifetime, Borman-Johnson model shows better agreement with experimental data. in the longer lifetime of the droplet over the steady-state period, the Abramzon-Sirignano model follows the trend of the experimental data and predictions are much closer to the measurements. So, Abramzon-Sirignano model has better compatibility with experimental data in longer droplet lifetimes than the other two models. Fig. 2 reveals that d-square law does not hold during droplet vaporization and therefore, the modified Spalding droplet vaporization model fails in estimating the non-dimensional droplet diameter. Fig. 3 shows the droplet vaporization rate during droplet lifetime. In the early period of the droplet lifetime, all mentioned evaporation models predict a very law Evaporation rate. After reaching the wet-bulb temperature, the predicted vaporization fluxes decrease for all evaporation models.

As shown in Fig. 1, the Abramzon-Sirignano model approaches the wet-bulb temperature. hence, in longer time; as it was indicated in Fig. 3, its distribution in mass flux is lower than the other two models. all models overpredict the evaporation rate and result in shorter droplet lifetimes. In Fig. 4, the variations of the non-dimensional square of droplet diameter with time for various droplet size are shown, using Abramzon-Sirignano model.



Fig. 2. variation of non-dimensional droplet diameter with respect to time



Fig. 3. variation of droplet vaporization rate with respect to time



Fig. 4. Comparison of the non-dimensional square of droplet diameter with respect to time under various droplet sizes using Abramzon-Sirignano evaporation model

As shown in Fig. 4 with decreasing the droplet diameter, the lifetime of the droplets decreases, because the small droplet requires a shorter time to evaporate than the large ones. It can also be seen that d^2 varies linearly with time following the d square law of Spalding. Fig. 5 shows the influence of ambient temperature on the surface temperature of a droplet. Three different ambient temperature of 800, 900, and 1000 K are selected.

As shown in Fig. 5 when the ambient temperature is increased, the steady-state temperature of the droplet will increase and the droplet reaches faster to wet-bulb temperature. Fig. 6 shows the influence of ambient pressures on the surface temperature of a droplet. Three different ambient pressures of 1, 5, and 10 atm are selected. The results of Fig. 6 indicates that increasing the ambient pressure increases the steady-state droplet temperature, also the ratio of the heat up time to the total vaporization time increases with increasing pressure. So, it follows that the evaporating characteristics of a droplet are very sensitive to the surrounding temperature and pressure.



Fig. 5. Comparison of the surface temperature of the droplet with respect to time at three different ambient temperature, using Abramzon-Sirignano evaporation model



Fig. 6. Comparison of the surface temperature of the droplet with respect to time at three different ambient pressures, using Abramzon-Sirignano evaporation model

Conclusions

Comparative analysis of three droplet evaporation models, namely the Spalding, Borman-Johnson, and Abramzon-Sirignano models, for a single fuel droplet are performed. Comparison with the experimental data indicates that the modified Spalding model fails to predict both droplet diameter and surface temperature. Results show that if Abramzon-Sirignano model is used, the surface temperatures and non-dimensional droplet diameter are in better agreement with experimental data than the other two models. Therefore, in this paper, this model is used for the parametric study of the effects of droplet size, ambient temperature and pressure on the droplet lifetime and temperature. Results indicate that by increasing the droplet size, the lifetime of the droplets will increase and the steady-state droplet temperature is higher at higher ambient pressures and temperature

Nomenclature

| Average physical properties fuel vapor/ air mixture in the gas film | $N_{mixture}$ |
|--|----------------------------|
| Correction factor | Z |
| Correction factor of the diffusional film thicknesses due to the Stefan flow | $F(B_M)$ |
| Correction factor of the thermal film thicknesses due to the Stefan flow | $F(B_T)$ |
| corrected Sherwood number | Sh^* |
| corrected Nusselt number | Nu* |
| Density | ρ |
| droplet diameter | d |
| fuel vapor mass fraction surface | У |
| Fuel vapor specific heat | $C_{_{PV}}$ |
| Heat penetrating into droplet | $Q_{\scriptscriptstyle L}$ |
| Latent heat of vaporization | L |
| non-dimensional parameter | ϕ |
| Nusselt number | Nu |
| Nusselt number (without Stefan flow effect) | Nu_0 |
| | |

| Molar fraction | x |
|-----------------------------------|-----------------|
| physical properties of air | N_{gas} |
| physical properties of fuel vapor | $N_{fuelvapor}$ |
| Pressure | Р |
| Spalding mass transfer number | B_{M} |
| Spalding heat transfer number | B_T |
| Temperature | Т |
| Thermal Conductivity | k |
| Time | t |
| vaporization rate | m |
| Subscript | |
| Droplet | d |
| Fuel vapor | F |
| Gas | g |
| Initial state | 0 |
| Liquid | l |
| Mean | m |
| Surface | S |

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