THE EFFECTS OF VARIABLE THERMOPHYSICAL PROPERTIES ON DROPLET EVAPORATION IN HIGH TEMPERATURE CONVECTIVE FLOW ENVIRONMENT

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Abstract - Evaporation of fuel droplets in a convective environment has significant applications in several energy systems, for example in internal combustion engines. Appropriate estimation of evaporation rate is critical in predicting performance of the system, which involves computation of the relevant heat and mass transfer terms. All of these terms are sensitive to the physical properties of the phases and affected by the transient variation of the corresponding phase temperature. In the present study, effects of temperature dependent thermo-physical properties of both liquid and gas phases on the evaporation behaviour of the droplet are investigated using a previously reported vaporization model (Nguyen et al., 2015) and compared with the available experimental data. Analysis shows that in a high temperature ambiance, use of temperature dependent thermo-physical properties for the gas phase and constant properties at an average temperature for the liquid phase produce the best agreement with experimental data.

Key words - evaporation, heat transfer, mass transfer, thermos-physical properties; average temperature.

1. Introduction

Droplet evaporation has many significant applications in several energy systems such as in internal combustion engines, gas turbines, liquid rocket engines, liquid fuel fired industrial furnace etc.

The fuel droplet evaporation models have been categorized into the following six groups with increasing level of complexity in computation (Sirignano, 2010): (1) constant droplet temperature models (2) infinite liquid thermal conductivity models; (3) finite liquid thermal conductivity models; (4) effective liquid thermal conductivity models where both the finite liquid thermal conductivity and the recirculation inside droplets are accounted; (5) vortex model where the recirculation inside droplets in terms of vortex dynamics is described; and (6) Navier-Stokes solution models where the complete solution of the flow field can be obtained. The 1st group of models assumes isothermal condition and neglects any temperature gradient inside droplet which enables related computations to be faster.Nonetheless, such assumption in the context of real application is over-simplified and may be inappropriate for droplets evaporating in a high temperature environment. In contrast, the fifth and sixth group models are computationally expensive even for single droplet calculations and often limited by the available computational resources for use in spray calculation (multi-droplet system). Models belonging to group (2), (3) and (4) have been used in droplet evaporation studies over several decades. Although simple, the infinite thermal conductivity (ITC) modelfrom 2nd group has been applied successfully in application like spray combustion (Chen and Periera, 1996) for its sufficient accuracy. Also, this model was previously revised and validated by Miller et al. (1998) and later by Nguyen et al. (2015) using experimental data of Ranz and Marshall (1952) and Downing (1966).

A major concern in the vapour-liquid equilibrium based evaporation models is the flow of droplet's vapour around interface, which significantly reduces the evaporation rate by preventing contact between fresh hot gas and the droplet. Since the introduction of the Frossling's empirical correlations in 1938, there have been several modified evaporation models to account for this vapour blowing effect (Stefan flow) in the modelsusing appropriate correction factors (Ranz and Marshall, 1952; Yuen and Chen,1976; Renksizbulutand Yuen., 1983; Miller et al., 1998; Sazhin et al., 2006).

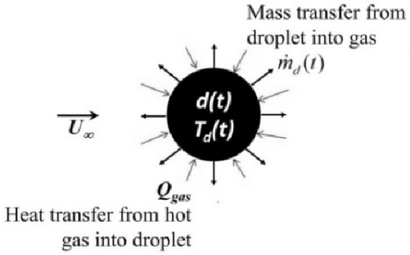

Figure 1. *A subcooled liquid droplet evaporating in hot gasstream*

Briefly, the evaporation process of a single subcooled droplet in a hot convective environment involves simultaneous heat transfer from gas to liquid phase and mass transfer from the liquid phase to gas phase (Fig.1). In a high temperature environment, gas phase temperature may be assumed to remain unchanged; however; temperature of both liquid and vapour mixture near interface will substantially increase during the evaporation process. Conversely, for a low temperature case, change in droplet and vapour mixture temperature is insignificant and therefore can be ignored. However, for a significant change in the liquid temperature due to a high gas temperature, dependence of the physical properties on temperature needs to be taken into account to determine the evaporation rate. The present study paper aims to investigate the effects of variable thermo-physical properties on the droplet evaporation in high temprature of the gas stream. Calculations in the present study are obtained by using the revised ITC model in which the modified Nu and Sh numbers suggested by Abramzon and Sirignano (1989) based on film theory are used to account for the Stefan flow.Details of the model can be found in the earlier study of the authors (Nguyen et al., 2015). The model is evaluated against the experimental data of Wong and Lin (1992) for a single decane droplet evaporating in high temperature of the ambient gas.

2. Model descriptions

Assuming spherical shape and uniform temperature in the entire liquid droplet,the transient temperature (T_d) and mass (m_d) of the droplet can be written as:

$$m_d C_{pL} \frac{dT_d}{dt} = \pi dNu / k_G \left(T_G - T_d\right) + L_v \dot{m}_d \qquad (1)$$

$$\dot{m}_d = \pi d \rho_G D_v Sh \ln\left(1 + B_M\right) \qquad (2)$$

The droplet diameter could be calculated either from the droplet evaporation rate$\dot{m}_d$or from the total droplet mass m_d simply as$d = \left(6m_d / \pi\rho_L\right)^{1/3}$ which is used in the present study. Thermodynamic liquid-vapour equilibrium state at the droplet surface is assumed and the Clausius-Clapeyron correlation is utilized to estimate the vapour pressure; mole and mass fraction of the vapour at the droplet interface. Substituting vaporization term from Eq.(2) into Eq.(1), Eq.(1) is integrated by a 4th order Rung-Kutta method in MATLAB (ver: 2013) to determine the transient temperature and diameter variation of the droplet. The time step size is selected based on the characteristic heating-up time, which is found to be smallest compared to other characteristic times. Temperature dependent liquid phase properties such as density (ρ_L), viscosity (μ_L), thermal conductivity (k_L) and heat capacity (C_{pL}) are computed using Peng-Robinson equation of state model in Aspen Properties package (V8.4).Binary diffusion coefficient (D_v) is obtained from the Chapman-Enskog formulation (ref). Vapour phase properties specifically heat capacity (C_{pv}) and latent heat of evaporation (L_v) and all physical properties of carrier gas are calculated at the wet bulb temperature correlation proposed by Miller et al. (1998) as follows:

$$T_{WB} = 137\left(T_B / 373.15\right)^{0.68} \log_{10}(T_G) - 45 \qquad (3)$$

3. Results and Discussions

The numerical results obtained from the model are evaluated against the experimental data of Wong and Lin (1992). This particular experimental research reports both the temporal squared diameter and temperature of a single decane droplet (d_0=2.0mm) evaporating in a very high temperature low Reynolds number ambiance (T_G=1000K, Re_{d0}=17 or U_G=1.0m/s). Unlike many other experimental studies where only the temporal reduction of droplet diameter is reported, data of Wong and Lin (1992) also comprises transient temperature measurement of the droplet, which allows a thorough evaluation of the models.

As the temperature of the liquid droplet varies during the vaporization process, the relevant physical properties such as density, heat capacity, thermal conductivity, viscosity, latent heat of vaporization and binary diffusion coefficient need to be computed at the corresponding temperature. The impacts of these variable physical properties on the evaporation time are investigated in the present study. First, the effects of the binary diffusion coefficient on the evaporation behavior are examined. Equation (2) indicates that binary diffusivity (D_v) is related to the vaporization rate of droplet which in turn affects the droplet temperature as can be found in Eq. (1). One can see that a higher value of diffusion coefficient results in a higher vaporization rate, which in turn predicts a lower droplet temperature. In this study D_v is estimated using the Chapman–Enskog theory based on the Lennard-Jones parameters obtained from four different sources (see Appendix). Temperature term in the expression of D_v is computed using the wet bulb temperature T_{WB}given in Eq.(3). Four different sources of Lennard-Jones parameters provide a wide range of D_v from 0.55 x 10^{-5} to 1.11 x 10^{-5} m^2/s. Figure 2 and Figure 3 compare droplet size and temperature using these four different diffusivity parameters. The largest deviation in the model prediction is ~ 2.5% for droplet lifetime (Fig. 2) and ~ 3.6% for droplet temperature (Fig. 3) which results in 11° difference. Results obtained by the largest D_v at 1.11 x 10^{-5} are found to agree with experimental data.

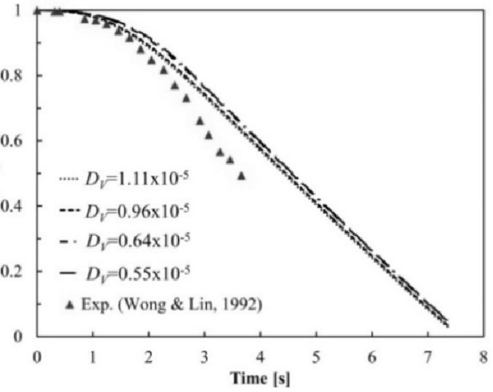

Figure 2. *Effects of the diffusion coefficient on the droplet size. Conditions are: T_{d0}=315K. T_G=1000K. T_B=447.1K. d_0=2mm. Re_{d0}=17*

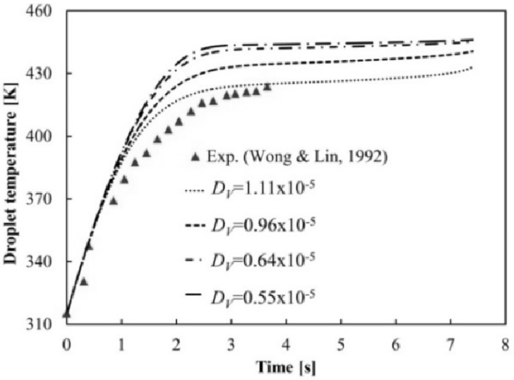

Figure 3. *Effects of the diffusion coefficient on the droplet temperature. Conditions of Fig. 2.*

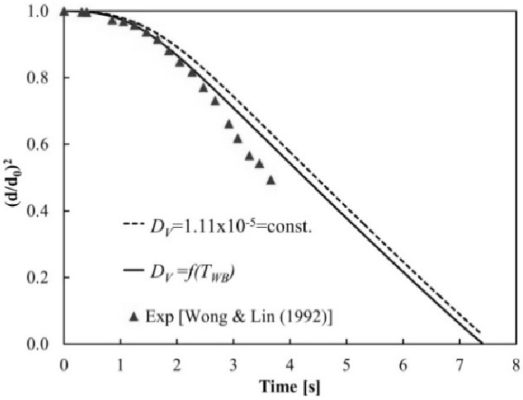

Figure 4. *Effects of the temperature dependent diffusion coefficient on droplet size. Conditions of Fig. 2.*

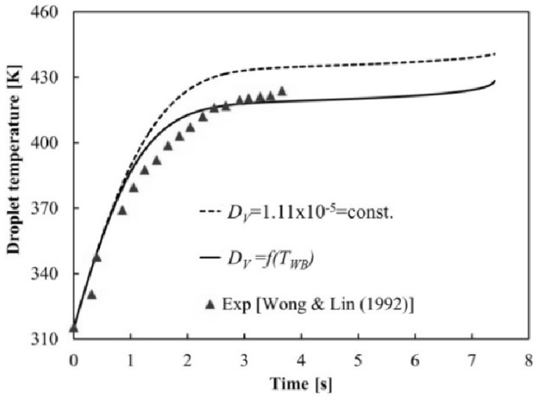

Figure 5. *Effects of the temperature dependent diffusion coefficient on droplet temperature. Conditions of Fig. 2.*

Figure 4 and Figure 5 present the droplet size and temperature profiles with the two different diffusion coefficient evaluation methods, i.e. $D_v=f(T_{WB})$ and $D_v=1.11 \times 10^{-5}$ (constant). Better agreement with experimental data is obtained when the temperature dependent D_v is used which results in NRMSD=0.10 for droplet size and NRMSD=0.06 for droplet temperature compared with constant D_v which yields an NRMSD=0.14 and 0.12 for droplet size and temperature respectively.

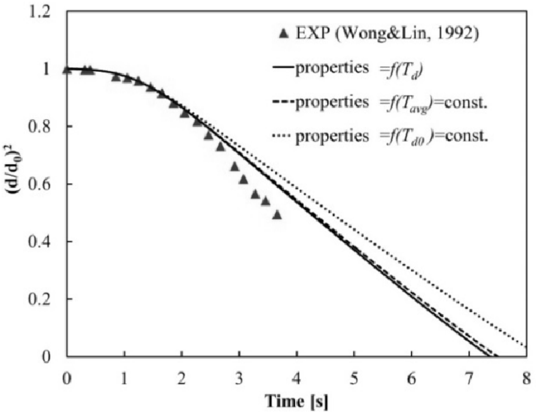

Figure 6. *Effects of the liquid properties on the droplet evaporation time. Conditions of Fig. 2.*

The effects of the liquid physical properties on the droplet lifetime are presented in Fig. 6. Relevant thermos-physical properties of liquid phase such as density, viscosity, thermal conductivity and heat capacity are estimated by three different methodologies: (1) at droplet temperature, T_d (base case); (2) at constant droplet temperature,T_{d0};and(3) at constant average droplet temperature, T_{avg}. The average temperature T_{avg} is obtained as $T_{avg}=0.5(T_{d0}+T_B)=381K$ (Abramzon&Sirignano, 1989) based on the assumption that droplet temperature will increase to boiling point from its initial temperature while evaporating in a high temperature environment. The evaporation time is found to be~ 12% larger when the liquid properties are evaluated at T_{d0}compared to the base case at T_d. Deviation in model prediction reduced to only ~ 2% when thermos-physical properties are estimated at T_{avg}. This insignificant difference suggests use of average temperature to estimate properties in the model for droplet evaporation in high temperature carrier gas. However, a caution is worth noting when carrier gas temperature is lower than the boiling point of droplet. Use of average temperature expression mentioned before in this case may lead to a lower value compared with the real average droplet temperature.

4. Conclusion

The effects of the thermo-physical properties of the gas and liquid phase are evaluated by using the revised infinite thermal conductivity model and published experimental data. For the gas phase (vapour mixture), calculations using temperature dependent binary diffusion coefficient provides a better agreement compared to constant diffusion coefficient. For the liquid phase, a deviation ~ 12% in the evaporation time are found as the physical liquid properties evaluated once at the droplet's initial condition whereas a negligible change in the evaporation time (~2%) as these properties are evaluated once at the temperature average temperature (compared to the base case of instantaneous temperature dependent properties). This study therefor concludes that temperature dependent properties for the gas phase and constant properties at the average temperature for the liquid phase should be used for the droplet evaporation calculations in high temperature environment to obtain better agreement with experimental data.

Notation

T temperature, *K*

U_∞ velocity of gas respecting to droplet, *m/s*

M molecular weight, *kg/kmol*

m mass, *kg*

d droplet, *m*

C_p heat capacity, *J/kgK*

$\dot{m}_d$ evaporation rate, *kg/s*

L_V latent heat of evaporation, *J/kg*

k thermal conductivity, *W/mK*

D_v diffusion coefficient of vapour into air, *m²/s*

$Sh=Kd_d/D_v$, (K is mass transfer coefficient)

$Nu=hd_d/k_G$, (h is heat transfer coefficient)

$\Pr = \mu_G C_{pG} / k_G$ Prandtl number of

$\mathrm{Re}_d = \rho_G U_\infty d_d / \mu_G$ Reynolds number of gas phase

Greek letters

μ viscosity, *Ns/m²*

ρ density,*kg/m³*

Subscripts

d Droplet

G gas

L liquid

V vapour

NRMSD: Normalized Root Mean Squared Deviation, itwas defined by ratio between the RMSD and the range of the measured data (maximum value minus minimum value).

APPENDIX

Physical properties of liquid Decane

Vapour (Abramzon&Sirignano, 1989)

$T_{WB}/1000 < 0.8$:

$$C_{pV} = 106.6 + 5765 \times T_{WB}/1000 - 1675 \times (T_{WB}/1000)^2 + 473.1 \times (T_{WB}/1000)^3$$

$T_{WB}/1000 \geq 0.8$:

$$C_{pV} = 411.1 + 5460 \times T_{WB}/1000 - 2483 \times (T_{WB}/1000)^2 + 422.9 \times (T_{WB}/1000)^3$$

Liquid (Aspen Properties V8.4)

$$\rho_L = -5.916 \times 10^{-4} T_d^2 - 3.974 \times 10^{-1} T_d + 8.982 \times 10^2, kg/m^3$$

$$C_{pL} = 9.428 \times 10^{-4} T_d^2 + 3.977 T_d + 8.088 \times 10^2, J/kgK$$

$$k_L = -1.678 \times 10^{-7} T_d^2 - 1.208 \times 10^{-4} T_d + 1.832 \times 10^{-1}, W/mK$$

$$\mu_L = -1.809 \times 10^{-10} \times T_d^3 + 2.292 \times 10^{-7} \times T_d^2 - 9.877 \times 10^{-5} \times T_d + 1.470958 \times 10^{-2}, \ Ns/m^2$$

Physical properties of (Aspen Properties V8.4)

$$\rho_G = -4.195 \times 10^{-9} \times T_{WB}^3 + 9.608 \times 10^{-6} \times T_{WB}^2 - 7.941 \times 10^{-3} \times T_{WB} + 2.79525, \ kg/m^3$$

$$C_{pG} = 2.632 \times 10^{-8} \times T_{WB}^2 + 1.764 \times 10^{-4} \times T_{WB} + 9.368 \times 10^2, J/kgK$$

$$k_G = -1.196 \times 10^{-8} \times T_{WB}^2 + 7.089 \times 10^{-5} \times T_{WB} + 4.812 \times 10^{-3}, W/mK$$

$$\mu_G = -5.982 \times 10^{-17} \times T_{WB}^4 + 1.608 \times 10^{-13} \times T_{WB}^3 - 1.542 \times 10^{-10} T_{WB}^2 + 1.029 \times 10^{-7} T_{WB} - 1.913 \times 10^{-6}, Ns/m^2$$

Binary diffusion coefficient of vapour in air

The binary diffusion coefficient of decane into air is estimated using the Chapman-Enskog theory as:

$$D_v = 1.8583 \times 10^{-7} \times \frac{\sqrt{T^3(1/M_V + 1/M_C)}}{p_C \sigma_{VC}{}^2 \Omega_{VC}}$$

where the pressure term p_c is equal to 1 atm.

The integral collision Ω_{VC} is calculated using the following correlation

$$\Omega_{VC} = \frac{1.06036}{T^{*0.1561}} + \frac{0.193}{exp(0.47635 \times T^*)} + \frac{1.03587}{exp(1.52996 \times T^*)} + \frac{1.76474}{exp(3.89411 \times T^*)}$$

$$T^* = T k_B/\varepsilon, \sigma_{VC} = 0.5(\sigma_V + \sigma_C), k_B = 1.38065 \times 10^{-23},$$

$$\varepsilon = \sqrt{\varepsilon_V \times \varepsilon_C}$$

The Lennard Jones potential model constants σ and ε/k_B of air are 3.711 and 78.6 respectively (Bird et al, 2007). σ and ε/k_B of the vapour (V) of four different sources are shown in Table 1.

Table 1. *Lennard Jones potential model constants of different sources for decane*

Sources	σ_v	ε_v/k_B	$D_v[m^2/s]$
Tavares (1997)	4.604	238.80	1.11E-05
Yu and Gao (2000)	5.233	226.46	9.64E-06
Parades et al (2000)-M1	6.563	456.74	6.44E-06
Parades et al (2000)-M2	7.164	572.56	5.49E-06

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