

Effect of temperature dependence of gas thermo-physical properties on analytical modelling of drop heating and evaporation

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Introduction

Heat and mass fluxes from an evaporating droplet in a gaseous mixture strongly depend on the evaluation of the transport and thermodynamic properties of both the gas and the liquid phases [1]. The majority of the available analytical models for drop vaporisation assume that transport properties are uniform through the gas phase, then neglecting their dependence on the local temperature and composition. The values of the properties are evaluated by an averaging procedure, and studies available in the open literature have shown that evaporation rate predictions are quite sensitive to the choice of property values.

Moreover, almost all analytical models available in the open literature used for dispersed spray applications assume a spherical shape for the evaporating drop, while experimental observations show that in dispersed phase scenarios, liquid drops are far from being spherical [2].

The objective of the present work is to show, through an analytical approach, the effect of temperature and composition dependence of gaseous mixture density, diffusivity, thermal conductivity and specific heat of the gas species on drop heat and mass transfer. The model is used for predicting, in analytic form, the evaporation and heating rates for different drop geometric configuration (ex. spheroidal drops, pair of spherical interacting drops).

Mathematical modelling

The heat and mass transfer from a finite bulk of liquid to the surrounding gas, under non-convective conditions, can be modelled using the species, energy and momentum conservation equations, which, under quasi-steady assumption, are expressed as

$$\nabla_j N_j^{(p)} = 0 \quad p = (0,1) \quad (1)$$

$$c_{p,v} \rho U_j \nabla_j T = \nabla_j (k_{mix} \nabla_j T) \quad (2)$$

$$\tilde{\nabla}_k \tilde{P}_T = \frac{1}{\Lambda} [Sc^M \tilde{\nabla}^2 \tilde{U}_k - \tilde{P}_T \tilde{T}^{-1} \tilde{\nabla}_j H \tilde{\nabla}_j \tilde{U}_k] \quad (3)$$

where $N_j^{(p)} = N_j^{(T)} y^{(p)} - c D_{10} \nabla_j y^{(p)}$ are the molar fluxes of the species p , according to the Fick's constitutive equations, $y^{(p)}$ is the molar fraction of the species p in the binary mixture, c is the molar density and D_{10} is the species diffusion coefficient. The indexes $p=(0,1)$ stand for the gas and the evaporating species, respectively, and $N_j^{(T)} = N_j^{(1)} + N_j^{(0)}$ is the j -component of the total molar flux. The energy equation (2) is reported in simplified form, which takes into account inter-diffusional terms, but neglects dissipation by viscous stresses and other minor terms (refer to [3, 4] for a more complete form of the equation); $c_{p,v}$ is the vapour heat capacity and k_{mix} is the thermal conductivity of the gaseous mixture. The momentum equation (3) is written in non-dimensional form, where $\tilde{\nabla} = R_d \nabla$ is the non-dimensional *nabla* operator and the following non-dimensional quantities have been introduced:

$$\tilde{P}_T = \frac{P_T}{c R T_\infty}; \quad \tilde{T} = \frac{T}{T_\infty}; \quad \Lambda = \frac{R T_\infty R_d^2}{M m^{(1)} D_{10}^2}; \quad \tilde{U} = U \frac{R_d}{D_{10}}; \quad Sc^M = \frac{\mu_{ref}}{D_{10} c M_m^{(1)}}; \quad H = \log(1 - y^{(1)}) \quad (4)$$

P_T is the ambient pressure, R is the universal gas constant, T_∞ is the gas temperature in the region of undisturbed flow, R_d is the equivalent volume drop radius, $M m^{(1)}$ is the molar mass of the vaporising species, U is the flow velocity. The parameter Λ in equation (3), for the operating conditions typical of spray applications, is orders of magnitude larger than the term in square brackets. This implies that the term on the right hand side of equation (3) is very small and the pressure field can be assumed constant and the momentum equation can be disregarded in the following analysis.

The species and energy conservation equations (1,2) form a coupled system of non-linear PDEs in the unknowns temperature, T , and molar fraction distribution, $y^{(p)}$. All the thermo-physical properties appearing in the equations (c , D_{10} , $c_{p,v}$, k_{mix}) are function of flow field temperature, pressure and composition. A fully analytical solution of the system, accounting for the temperature dependence of the thermo-physical properties, was recently proposed in [5]. Following a procedure suggested by [6], an auxiliary harmonic function Φ that satisfies the Laplace equation

with uniform boundary conditions is introduced and the system is solved in the natural curvilinear coordinate system of the problem. The heat and mass fluxes at the drop surface can then be calculated from the gradient of the function Φ (see [5]). The classical case, when all the thermo-physical properties are assumed constant, can be seen as a special case; the evaluation of the vapour and energy local mass fluxes reduces to the relations

$$n_n^{(1)} = -\rho_{ref} D_{10,ref} \ln(1 + B_M) \nabla_n \Phi \quad (5)$$

$$q_n = -k_{mix} T_\infty \nabla_n \Phi \quad (6)$$

where B_M is the Spalding mass transfer number

$$B_M = \frac{\chi_s^{(1)} - \chi_\infty^{(1)}}{1 - \chi_s^{(1)}} \quad (7)$$

$\nabla_n \Phi$ is the component normal to the drop surface of the gradient of the auxiliary function Φ and the properties are evaluated at a reference temperature and composition according to the expressions

$$T_{ref} = \alpha_{ref} T_\infty + (1 - \alpha_{ref}) T_s; \quad \chi_{ref}^{(p)} = \alpha_{ref} \chi_\infty^{(p)} + (1 - \alpha_{ref}) \chi_s^{(p)} \quad (8)$$

where χ is the mass fraction of the species p . In the classical models usually implemented in CFD codes for dispersed phase calculation, refer to [1] for the most common ones, the averaging parameter α_{ref} is a constant and results from the scientific literature [1, 7] suggest that the value of α_{ref} equal to $1/2$ should be used in case of low evaporating conditions, while the value equal to $1/3$ should be preferred under high evaporating conditions.

It has been shown [5] that the use of equations (5) and (6) can yield more accurate results if α_{ref} is evaluated as function of B_M . Taking advantage of the general model above described, the following correlation was suggested in [5]

$$\alpha_{ref} = \frac{A_{\alpha,ref}}{\log(1 + B_M)} + \frac{1}{1 - (1 + B_M)^{\frac{1}{A_{\alpha,ref}}}} \quad (9)$$

where the constants $A_{\alpha,ref}$ depends on the species and the gas temperature [5].

The effect of the modelling of thermo-physical properties on the evaporation of drops in stagnant gaseous environment is discussed in the following section for different liquids and drop shapes and configurations.

Results and discussion

This section reports a sample of the results from the investigation on the effect of the modelling of thermo-physical properties on the drop evaporation. The model accounting for the detailed dependence on temperature and composition of physical properties, which mathematical derivation is presented in [5], has been compared with the classical model, equation (5), where the properties are assumed constant at a reference temperature and gas mixture composition, according to equations (8). Different values for the averaging parameter α_{ref} have been used to show their effect of the evaporation rate predictions. Figure 1 reports the evaporation rate ratio γ , calculated as the ratio between the evaporation rate assuming constant physical properties and the evaporation rate assuming that the properties are function of temperature and composition. The non-dimensional evaporation rate is plotted as function of the Spalding mass transfer number for three fluids (n-octane, acetone and ethanol), which have been used for their different volatility and applications, where the liquid temperature has been varied from 280K up to the boiling temperature of the species and the gas temperature at free stream conditions has been assumed constant equal to 1000K. The three curves in each graph correspond to the different selection of the averaging parameter α_{ref} using the classical model: the constant values $1/3$ and $1/2$ have been selected as suggested in the literature, corresponding to the red and blue curves, respectively, while the black curve corresponds to the case where the averaging parameter is a function of the evaporating conditions, according to equation (9), and reported in the bottom graphs of Figure 1. The results confirm that for all the three fluids a value of the averaging parameter close to $1/2$ works well at low evaporating conditions (low $B_{M,l}$), while lower values of α_{ref} yield better approximation increasing the drop temperature (i.e. high $B_{M,l}$), although the value of $1/3$ commonly used in evaporation models for dispersed phase calculation may be still too high, particularly for n-octane and ethanol where values down to about 0.2 yield the best approximation as the drop temperature approaches the boiling point. The evaporation rate predicted using as averaging parameter the correlation (8) differs by less than 4% from the detailed model that assumes temperature dependent physical properties for all the operating conditions [5].

Figures 2 and 3 report the distribution of the vapour fluxes on the surface of water drops at two temperatures, equal to 339.5K and 369K, which correspond to moderately low and high evaporating conditions, respectively, vaporising in air at 1000K. The effect of modelling the physical properties is shown, and the vapour fluxes are calculated assuming constant physical properties according to equation (5). The constant values equal to $1/3$, $1/2$ and the values from the correlation (8) are selected and the corresponding vapour mass fluxes distributions are plotted in figure 2 for two spheroidal drops with surface area equal to $4\pi R_d^2 \beta$ (where β accounts for deformation

from spherical shape [7]) with β equal to 1.1. Figures 2(a,b) show the fluxes for the prolate drop shape, with the aspect ratio [8] $\varepsilon=2.22$, while figures 2(c,d) show the corresponding fluxes for the oblate drop shape, with the aspect ratio $\varepsilon=0.49$. The red arrows and the red contour represent the vapour fluxes fixing α_{ref} equal to $1/3$, the blue colour corresponds to the test cases with α_{ref} equal to $1/2$, while the black colour to the test cases with α_{ref} from equation (7). The graphs show the simultaneous effect of the drop shape and physical property calculation on the vapour fluxes, which are higher where the drop curvature is higher and viceversa and confirm that for water drops under low evaporating conditions the value of α_{ref} equal to $1/2$ can be used, while under high evaporating conditions the use of $\alpha_{ref}(B_M)$ given by equation (9) yields more accurate results.

The effect of the averaging parameter is shown for a different drop configuration in figure 3, with two identical drops at a distance equal to $4R_d$ [9], under the same operating conditions of figure 2. The graphs enlighten the effect of drop interaction on the vapour flux distribution, showing the screening effect on the evaporation due to the presence of the neighbouring drop. The dependence of the prediction on the choice of the averaging parameter is still noticeable, confirming the previous comments on the use of α_{ref} as a function of the operating conditions.

These results confirm the clear advantage of using a simple correlation for the property averaging parameter, which accounts for the dependence on temperature and composition of the thermo-physical property. Further investigation is required to improve the correlation for a wide range of fluids and operating conditions.

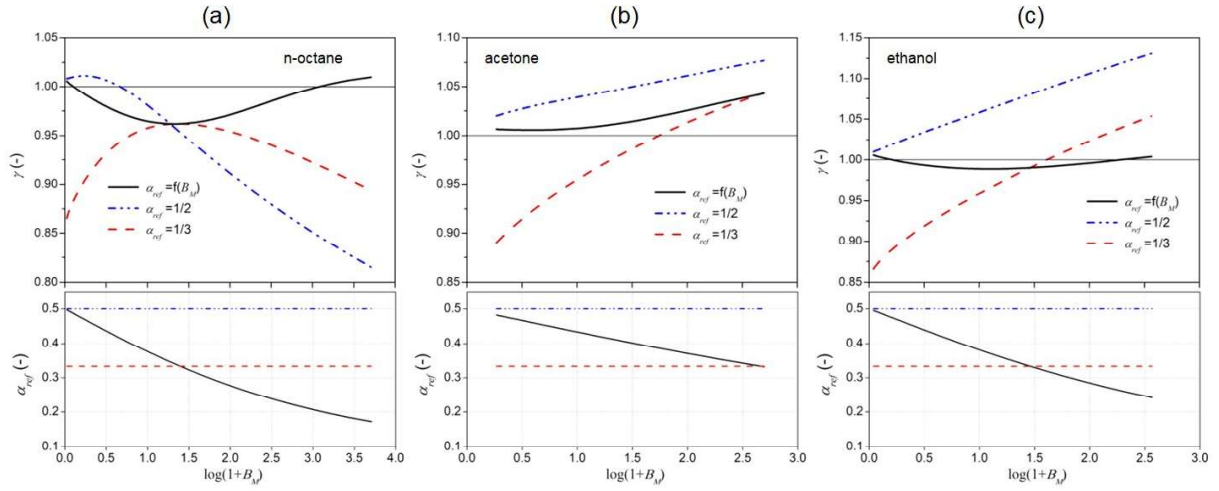


Figure 1. Evaporation rate ratio γ , as function of the Spalding mass transfer number, calculated using α_{ref} from Eq. (9) (solid black line), $\alpha_{ref}=1/2$ (dashed-dot green line) and $\alpha_{ref}=1/3$ (dashed red line), for n-octane drop in air at (a) 500 K and (b) 1000 K. The bottom graphs report Eq. (9) for each fluid.

Nomenclature

$A_{\alpha_{ref}}$	Averaging parameter constant [-]	$n^{(p)}$	mass flux of species p [kg m ² s ⁻¹]
B_M	Spalding mass transfer number [-]	$N^{(p)}$	Molar flux of species p [mol m ² s ⁻¹]
c	Molar density [mol m ⁻³]	P	Pressure [Pa]
$c_{p,v}$	Heat capacity at constant pressure [J kg ⁻¹ K ⁻¹]	R	Universal gas constant [J mol ⁻¹ K ⁻¹]
D_{10}	Mass diffusivity [m ² s ⁻¹]	R_d	Drop radius [m]
k	Thermal conductivity [W K ⁻¹ m ⁻¹]	T	Temperature [K]
m_{ev}	Evaporation rate [kg s ⁻¹]	U	Velocity [m s ⁻¹]
M_m	Molar mass [kg kmol ⁻¹]	y	Molar fraction [-]
Greek symbols		ρ	Mass density [kg m ⁻³]
α_{ref}	Averaging parameter [-]	Φ	Harmonic function [-]
β	Surface area ratio [-]	χ	Mass fraction [-]
γ	Evaporation rate ratio [-]		
Subscripts		T	Total [-]
mix	Mixture [-]	∞	Free stream conditions [-]
ref	Reference conditions [-]		
s	Surface [-]		

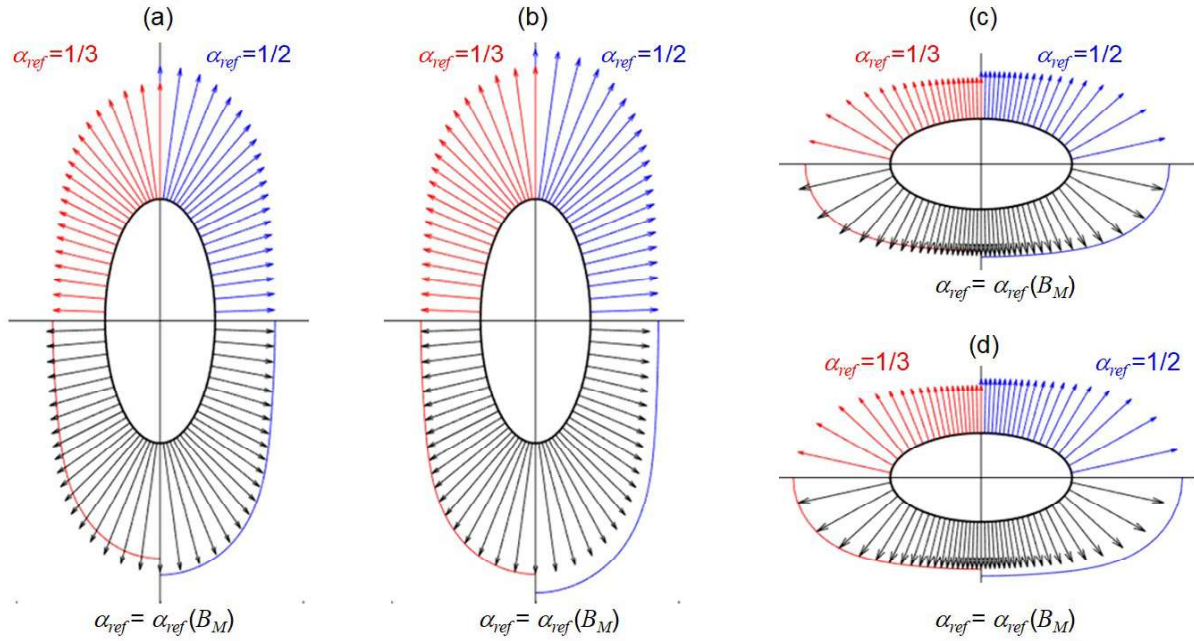


Figure 2. Effect of averaging parameter α_{ref} on the surface vapour flux distribution of spheroidal water drops with $\beta=1.1$ ($\varepsilon=2.22$ for prolate and $\varepsilon=0.49$ for oblate drops) vaporising in air at $T_\infty=1000\text{K}$; (a) prolate drop at $T_s=339.5\text{K}$, (b) prolate drop at $T_s=369\text{K}$, (c) oblate drop at $T_s=339.5\text{K}$, (d) oblate drop at $T_s=369\text{K}$.

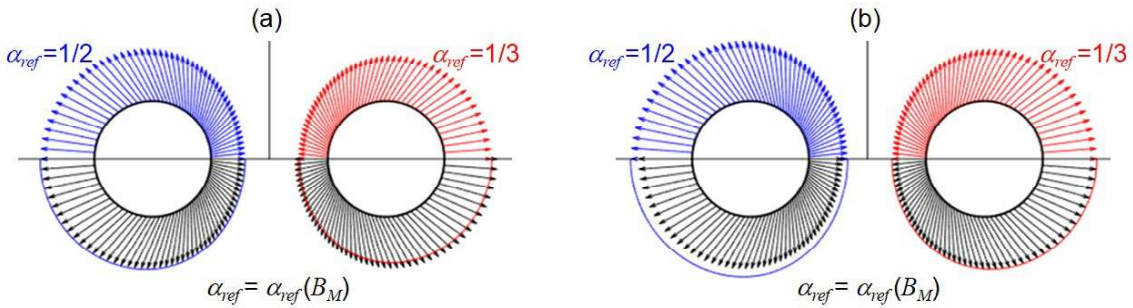


Figure 3. Effect of averaging parameter α_{ref} on the surface vapour flux distribution of two interacting water drops with distance equal to $4R_d$ vaporising in air at $T_\infty=1000\text{K}$; (a) $T_s=339.5\text{K}$, (b) $T_s=369\text{K}$.

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