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Mass transfer from a drop—II. Theoretical analysis of temperature dependent mass flux correlation

MARKKU KULMALA and TIMO VESALA
Department of Physics, P.O. Box 9, FIN-00014 University of Helsinki, Finland

and

JAROSLAV SCHWARZ and JIRI SMOLIK
Institute of Chemical Process Fundamentals, Academy of Sciences of the Czech Republic,
Rozvojova 135, 165 02 Prague 6, Czech Republic

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Abstract—A new expression of the droplet Sherwood number (*Sh*) is presented based on the theoretical treatment of the temperature dependent gaseous diffusion coefficient. The experimentally specified parameters were correlated by means of recent data on water droplets evaporating in the flow field. The mass flux correlation is given as a function of the Reynolds (*Re*) and Schmidt (*Sc*) numbers, and it turned out to be $Sh = (2.009+0.514Re^{1/2}\,Sc^{1/3})$. The Sherwood number should be multiplied by a strictly theoretical correction factor which depends on the droplet and gas temperatures and which is order of 0.9, if the temperature deviation is order of 100 K. The introduction of the correction factor seems to remove a discrepancy existing between the earlier theoretical treatments and experimental data.

INTRODUCTION

Evaporation of drops is a process, which is important in many industrial (e.g. combustion, spray drying, wet scrubbing) and atmospheric processes (e.g. releases of hazardous materials, evaporation of rain droplets). The evaporation is determined by simultaneous mass and energy transfer. If the surrounding gas is moving with respect to a droplet, the diffusive rates of mass and heat transfer from the droplet surface are increased. The convective transfer may be due to the relative velocities of the gas and droplets (forced convection) or due to density gradients (free convection).

In the present paper we present a new expression for the droplet Sherwood number due to forced convection. The expression is based on the theoretical treatment of diffusive mass transfer in the continuum regime and it includes the Stefan flow [1, 2]. The fitting of correlation parameters in the Sherwood number is done using the recent experimental data on the mass flux of an evaporating water droplet [3].

THEORY

In order to calculate droplet evaporation, it is necessary to determine the gas-phase mass flux density (the rate at which mass of species passes through a unit cross section placed perpendicular to the velocity of species) and the actual droplet temperature. In this study we will not consider the methods to estimate the droplet temperature; we treat the mass flux density expression assuming that the temperature is known. For a single component droplet in the convective-free case, the continuum regime expression is well-known, originating from the Stefan–Maxwell equations [4]. On the contrary, only some general mathematical solutions for forced convective transfer around droplets are available [5–8] because of the changes of flow characteristics with droplet Reynolds number. For that reason one usually applies the diffusive mass flux expression (giving the rate at which mass of species is transferred from a droplet surface) corrected semi-empirically for forced convection, i.e. the diffusive mass flux is multiplied by the droplet Sherwood number. However, in order to obtain algebraic expression for the diffusive mass flux, the mass flux density expression must be integrated. The correct temperature dependence of the gaseous diffusion coefficient is normally neglected in the integration, but it can be very significant as will be shown below.

Diffusive mass flux

We present briefly the derivation of the diffusive mass flux expression for a spherical droplet contained in an infinite volume of a tranquil inert gas. The expression includes the correct temperature dependence of the gaseous diffusion coefficient (for more details see ref. [1]; see also ref. [2]).

NOMENCLATURE

a	droplet radius
c	molar density of gas
C	correction factor resulting from temperature dependent diffusion coefficient
D	binary diffusion coefficient
I	mass flux
$\vec{j}_{\mathrm{v}}$	mass flux density
M_{v}	molecular weight of vapor
p	total gas pressure
p_{v}	partial vapor pressure
r	radial distance
R	universal gas constant
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
T	temperature
x_{v}	mole fraction of vapor.

Greek symbols

α, β	fitting parameters for Sherwood number
μ	coefficient for temperature dependence of diffusion coefficient.

Subscripts

a	value at droplet surface
∞	value far from droplet.

In the absence of a gradient in the total pressure and in the absence of external forces, the mass flux density resulting from ordinary molecular diffusion is given by (see refs. [2, 4, 9, 10])

$$\vec{j}_{\mathrm{v}} = -\frac{DM_{\mathrm{v}}p}{RT(1-p_{\mathrm{v}}/p)}\nabla(p_{\mathrm{v}}/p). \qquad (1)$$

Here vapor and inert gas are assumed to be ideal, i.e. the ratio of the partial pressure of vapor (p_{v}) to the total pressure (p) is equal to the mole fraction of vapor. M_{v} is the the molecular weight of vapor and R is the general gas constant. The binary diffusion coefficient D depends on temperature T approximately by [11]

$$D(T) = D_{\infty}(T/T_{\infty})^{\mu} \qquad (2)$$

where D_{∞} is the diffusion coefficient at the temperature T_{∞} far from the droplet (this reference temperature is chosen for convenience). The coefficient μ varies in most cases from 1.5 to 2.0 [11] and over small temperature ranges it can be assumed constant. Note that the binary diffusion coefficient is virtually independent of composition.

For stationary mass transfer $\nabla \cdot \vec{j}_{\mathrm{v}} = 0$ and the constant mass flux can be readily identified as

$$I = -4\pi r^2 \frac{D(T)pM_{\mathrm{v}}}{(1-p_{\mathrm{v}}/p)RT}\frac{\mathrm{d}(p_{\mathrm{v}}/p)}{\mathrm{d}r} \qquad (3)$$

where r is the radial distance. The mass flux is normally estimated by integrating the above expression over r and p_{v} and by assuming the gas temperature (and D) as constant (see ref. [9]). In this approach the temperature is often set equal to T_{∞} and D is estimated also at T_{∞} or at the geometric mean $\sqrt{(T_{\infty}T_{\mathrm{a}})}$ [12], where subscript a refers to the value at the droplet surface. However, if the temperature deviation between the droplet surface and the infinity is several tens of degrees Kelvin its effect starts to be considerable [2] and a more correct form of the temperature dependence is desired.

The effect of the temperature deviation can be analytically estimated using the hyperbolic temperature profile

$$T = T_{\infty} + (T_{\mathrm{a}} - T_{\infty})\frac{a}{r}. \qquad (4)$$

This expression is a bit inaccurate, assuming implicitly a constant thermal conductivity and a constant vapour enthalpy [2] (see also refs. [10] and [13]), but it offers a straightforward method to replace r-dependence by T-dependence in equation (3); namely

$$\frac{\mathrm{d}r}{r^2} = -\frac{\mathrm{d}T}{a(T_{\mathrm{a}} - T_{\infty})}. \qquad (5)$$

Substituting this into equation (3) and separating of variables we obtain

$$\frac{IR}{4\pi a M_{\mathrm{v}}(T_{\mathrm{a}} - T_{\infty})}\int_{T_{\mathrm{a}}}^{T_{\infty}} \mathrm{d}T\frac{T}{D(T)} = p\int_{a}^{\infty}\frac{\mathrm{d}(p_{\mathrm{v}}/p)}{1-p_{\mathrm{v}}/p}. \qquad (6)$$

Using equation (2) the integration gives

$$I = -\frac{4\pi a p M_{\mathrm{v}} D_{\infty} C}{RT_{\infty}}\ln\frac{1-p_{\mathrm{va}}/p}{1-p_{\mathrm{v}\infty}/p} \qquad (7)$$

where

$$C = \frac{T_{\infty} - T_{\mathrm{a}}}{T_{\infty}^{\mu-1}}\frac{2-\mu}{T_{\infty}^{2-\mu} - T_{\mathrm{a}}^{2-\mu}} \qquad (8)$$

if $\mu \neq 2.0$ and

$$C = \frac{T_{\infty} - T_{\mathrm{a}}}{T_{\infty}\ln\dfrac{T_{\infty}}{T_{\mathrm{a}}}} \qquad (9)$$

if $\mu = 2.0$. The behaviour of these expressions in different cases (for example, $T_{\mathrm{a}} \to T_{\infty}$) is discussed in ref. [2]. Note that if the Stefan flow is neglected the logarithmic term in equation (7) reduces only to a difference of vapor pressure ratios.

The Sherwood number

Different definitions for the average droplet Sherwood number have been presented by various authors. The effect of the Stefan flow has been often neglected (e.g. ref. [14]) or it has been approximately included using slow mass-transfer rate assumption (e.g. refs. [4, 15, 16]). Renksizbulut *et al.* [17] corrected empirically the Sherwood number for high mass-transfer rate (blowing effect). Downing [18] included the correct form of the Stefan flow in the definition of the Sherwood number and he introduced also a temperature dependent empirical correction. Schwarz and Smolik [3] have compared their own experimental results with the different definitions mentioned just above.

According to equations (7) and (8) or (9), we define the Sherwood number as

$$Sh = \frac{I}{C 2\pi a c_\infty D_\infty \ln((1-x_{va})/(1-x_{v\infty}))} \qquad (10)$$

where c_∞ is the molar density far from the droplet and x_{va} and $x_{v\infty}$ are the vapor mole fractions at the droplet surface and far from the droplet, respectively. In the absence of forced convection Sh is equal to 2 by definition. Note that the above expression is similar to that of Downing [18] who introduced the experimental correction factor instead of the factor C.

RESULTS AND DISCUSSION

To make the correlation for the Sherwood number we used recent data obtained by Schwarz and Smolik [3] for water droplet evaporation. They presented 186 experimental points for the mass flux in the Reynolds number range ($30 < Re < 180$) when the gas temperature varied from 314 to 449 K and the measured droplet temperature varied from 287 to 315 K. The free stream velocity varied from 0.5 to 1.7 m s^{-1} and the drop diameter from 0.7 to 2.3 mm [3].

For the intermediate Reynolds number range, as here, theoretical and experimental results suggest that [14–16]

$$Sh = \alpha + \beta\, Re^{1/2}\, Sc^{1/3} \qquad (11)$$

where Sc is the Schmidt number. The parameter α should be near to 2 from the requirement of the consistent theory. The Reynolds and Schmidt number include some thermophysical properties of gas mixture which should be evaluated at an appropriate reference temperature $T_{r,i}$ and composition $p_{vr,i}$. Typically $T_{r,\infty} = T_\infty$ or $T_{r,1/2} = T_a + 1/2(T_\infty - T_a)$ or $T_{r,1/3} = T_a + 1/3(T_\infty - T_a)$ with the respective definitions for $p_{vr,i}$. The thermophysical properties needed for correlations were adopted from refs. [19] and [20]. The coefficient μ was 1.8 [19] and the correction factor C, equation (8), varied from 0.86 to 0.98.

By correlating the data of Schwarz and Smolik [3] with equations (10) and (11), we discovered that

$$Sh = 2.009 + 0.514 Re^{1/2}\, Sc^{1/3} \qquad (12)$$

with the correlation coefficient of 0.94. The plot of this formula and the experimental data are presented in Fig. 1. The correlation indicates a good fit of the data and it predicts well the theoretical interception value of 2. For the thermophysical properties $T_{r,i} = T_{r,1/3}$ and $p_{vr,i} = p_{vr,1/3}$ were used (see also refs. [21] and [22]), but we also tried other definitions. Their accuracy was almost as good as that of the $T_{r,1/3}$ and $p_{vr,1/3}$ correlations.

The regression equation obtained here agrees well with previous results. The coefficient β is close to the value (0.552) obtained by Frössling [14]. Downing [18] presented the temperature dependent correction factor for the Sherwood number with $\beta = 0.6$. His strictly empirical correction $1 - 0.4(1 - T_\infty/T_a)$ is quite close to the our theoretical correction C in the conditions considered in this study. Finally, Wedding *et al.* [23] presented the regression formula with $\alpha = 1.755$ and $\beta = 0.535$, and concluded that since the intercept value is significantly less than 2 there is an anomaly between theory and experimental data. However, when we made a new correlation with the correction factor C set to unity, the formula was found to be

$$Sh = 1.738 + 0.479 Re^{1/2}\, Sc^{1/3}. \qquad (13)$$

The fitting is still very good (the correlation coefficient was 0.93), but the value of the parameter α is inconsistent and close to that of Wedding *et al.* [23]. Note however that Wedding *et al.* have calculated the thermophysical properties at infinity, while with $C = 1$ we have calculated the gaseous molar density and the diffusion coefficient at infinity and Re and Sc by using 1/3 rule.

CONCLUSIONS

The new correlation for the droplet Sherwood number has been presented in the intermediate Reynolds number range. It includes the explicite temperature dependence of the diffusion coefficient and offers a clear physical background for mass transfer at high-temperature conditions. The intercept value at $Re \to 0$ given by the fit is practically the theoretical lower limit (2) for Sh. The correlation is based on data of

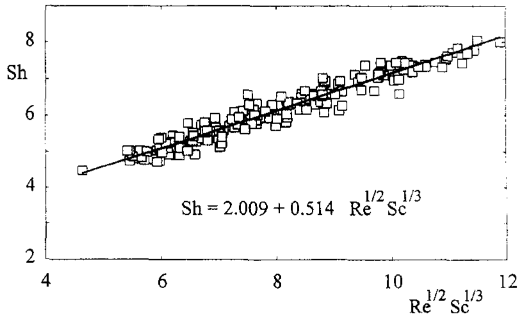

Fig. 1. Correlation of the experimental data [3] according to equation (10).

Schwarz and Smolik [3], including the droplet temperatures measured by a thermocouple 25 μm in diameter. Since the exact magnitudes of the presence of the capillary, the water adding and the thermocouple on droplet heat exchange processes are not known, any new information on the droplet Nusselt number can not be deduced from the used data. In the future the new correlation should be verified in the conditions of larger temperature deviation, stronger Stefan flow and smaller Reynolds numbers.

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