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To cite this article: Tarek Beji and Bart Merci 2018 J. Phys.: Conf. Ser. 1107 062002

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A Detailed Investigation on the Effect of the Sherwood and Nusselt Number Modelling for the Heating and Evaporation of a Single Suspended Water Droplet

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ABSTRACT
The work described in this paper presents a comprehensive analysis of the convective heat and mass transfer coefficient modelling around a single water droplet using an in-house code. The most widely used approach is to rely on sub-models for the non-dimensional heat and mass transfer numbers (called hereafter the Nusselt, Nu, and the Sherwood, Sh, numbers) and which are shown to take the theoretical and functional form of
\[ \text{Nu} = 2.0 + K_1 \text{Re}_d^{1/2} \text{Pr}^{1/3} \] and \[ \text{Sh} = 2.0 + K_1 \text{Re}_d^{1/2} \text{Sc}^{1/3} \] where \( \text{Re}_d \) is the droplet Reynolds number, \( \text{Pr} \) and \( \text{Sc} \) are the Prandtl and Schmidt numbers of the surrounding gas and \( K_1 \) and \( K_2 \) are constants. This formulation, which is generally referred to in the literature as the Ranz-Marshall model (with \( K_1 = K_2 = 0.6 \), is the most used approach in Computational Fluid Dynamics (CFD) codes for fire safety engineering. In this paper, we first assessed this formulation based on 36 experimental tests carried out in [Volkov and Strizhak, Applied Thermal Engineering (2017)] and where a single suspended water droplet of a diameter between 2.6 and 3.4 mm is heated up by a convective hot air flow with a velocity between 3 and 4.5 m/s and a temperature between 100 and 800°C. The results showed that the overall model uncertainty in the droplet lifetime prediction is about 34% with particularly poor results when the air temperature is 100 or 200°C. The droplet saturation temperatures were overestimated by around 20 to 30°C. After this initial assessment, we performed a sensitivity analysis and selected a combination of values for \( K_1 \) and \( K_2 \) that provided an overall simultaneous good agreement for both the droplet lifetimes (model uncertainty of 5%) and the droplet saturation temperatures (around 10°C). This analysis showed that, for high air temperatures (i.e., \( T_a \geq 300°C \)), the value of \( K_2 = 0.6 \) remains suitable. However, for these cases, the value of \( K_1 \) needed to be increased (to 1.8 and up to 4) in order to promote the evaporation-induced cooling and improve the predictions in terms of droplet saturation temperatures. For \( T_a = 100°C \), the ‘best’ combination was found to be \( K_1 = K_2 = 1.8 \). Such combination allowed to reduce the initially overestimated droplet lifetimes by promoting mass transfer (through an increased value of \( K_1 \)) without slowing down the heating process that generates water vapor at the droplet surface (explaining the equally increased value of \( K_2 \)). The case of \( T_a = 200°C \) appeared to be an intermediate case. The present results indicate that the ‘classical’ Ranz-Marshall approach with \( K_1 = K_2 = 0.6 \) is not optimal. A more thorough analysis, with eventually additional experimental data, is required.

KEYWORDS: water droplet; heat transfer; mass transfer; evaporation.
INTRODUCTION

An accurate water heating and evaporation model is essential for the assessment of the efficiency of active fire protection measures that are based on, for example, Early Fire Suppression Response (EFSR) sprinklers or water mist. Several correlations have been developed in the literature to estimate the convective heat and mass transfer film coefficients around droplets. The most widely used approach is to rely on sub-models for the non-dimensional heat and mass transfer numbers, namely the Nusselt, Nu, and the Sherwood, Sh, numbers, which are shown to take the theoretical and functional form of [1]:

\[
\begin{align*}
\text{Nu} &= 2.0 + K_1 \text{Re}_d^{1/2} \text{Pr}^{1/3} \\
\text{Sh} &= 2.0 + K_1 \text{Re}_d^{1/2} \text{Sc}^{1/3}
\end{align*}
\]  

(1)

where \( \text{Re}_d \) is the droplet Reynolds number, \( \text{Pr} \) and \( \text{Sc} \) are respectively the Prandtl and Schmidt numbers of the surrounding gas and \( K_1 \) and \( K_2 \) are constants. This formulation, which is generally referred to in the literature as the Ranz-Marshall model with \( K_1 = K_2 = 0.6 \) [1], is the most used approach in Computational Fluid Dynamics (CFD) codes for fire safety engineering. A myriad of similar correlations have been proposed in the literature [2-3] by modifying the coefficients \( K_1 \) and \( K_2 \), as well as the constant term 2, although the latter is suggested in [1] to remain unchanged in order to be consistent with the theoretical requirement of \( \text{Nu} = 2 \) and \( \text{Sh} = 2 \) at \( \text{Re}_d = 0 \). The variety of the proposed coefficients stems essentially from the change in experimental conditions such as the nature of the experimental test (e.g., suspended or free-fall single droplet) or the velocity and temperature of the convective hot air flow. To the best of the authors’ knowledge, most of the experimental studies on the evaporation of single water droplets in a hot environment are limited to ‘moderate’ free air stream temperatures, up to around 350°C (e.g., in [4]). However, very recently (in 2017), an experimental study have been reported on the heating and evaporation of a single suspended water droplet in a hot air environment with temperatures between 100 and 800°C [5]. The high temperatures considered therein represent a strong element of novelty and are particularly relevant for fire suppression applications. The objective of this paper is to develop an in-house code and rely on the dataset displayed in [5] in order to examine the accuracy of the numerical predictions depending on the choice for the values of \( K_1 \) and \( K_2 \) in Eq.(1).

NUMERICAL MODELLING

In this section the governing equations for mass and heat transfer are described along with the solution procedure that is used in the development in the in-house code.

Mass transfer

The evaporation rate of a spherical liquid droplet is expressed according to the Stefan-Fuchs model [2] as:

\[
\frac{d m_s}{dt} = \pi d_s \frac{k_m}{L_e} \frac{k_{m}}{c_{p,v}} \text{Sh} \ln\left(1 + B_M\right)
\]

(2)

where \( d_s \) is the droplet diameter, \( L_e \) is the Lewis number (taken as \( L_e = 1 \)), \( k_m \) is the mass weighted thermal conductivity of the mixture of water vapor and air at the air temperature and \( c_{p,v} \) is the specific heat capacity of water vapor at constant pressure and droplet surface temperature. The variable \( B_M \) denotes the Spalding mass transfer number expressed as [2]:

\[
B_M = \frac{Y_{v,s} - Y_{v,g}}{1 - Y_{v,s}}
\]

(3)

where \( Y_{v,s} \) is the mass fraction of the vapor at the liquid surface (calculated using the Clausius-Clapeyron equation) and \( Y_{v,g} \) is its mass fraction in the surrounding gas.

Heat transfer

Based on the assumption of uniform temperature, \( T_{sk} \) across the droplet diameter, the energy conservation equation for the spherical liquid droplet reads:
\[
\frac{dT_d}{dt} = \frac{1}{\tau} \left[ \alpha_1 \left( T_s^a - T_d \right) + \left( T_s - T_d \right) - \alpha_2 \ln \left( 1 + B_d \right) \right]
\]  

(4)

with

\[
\tau = \frac{\rho_d d_d^2 c_{p,d}}{6 k_m Nu}, \quad \alpha_1 = \frac{d_d c_{p,d} \sigma F_d}{k_m Nu}, \quad \alpha_2 = \frac{Sh}{Nu Le} \frac{1}{c_{pr}}
\]  

(5)

where \( \rho_d \), \( c_{p,d} \), \( \epsilon_d \) and \( L_n \) are respectively the density, specific heat, emissivity and sensible heat of vaporization of water and \( F_d \) is the view factor of the droplet (taken here as \( F_d = 0.5 \) [6]). The variables \( t \) and \( \sigma \) denote the time and the Stefan-Boltzmann constant.

Solution procedure

Similarly to [7], the heat transfer equation, i.e., Eq.(4), in combination with Eq.(2) for mass transfer, is discretized in time using a Crank-Nicolson scheme, along with a linearization of the radiation and natural logarithm terms using Taylor series.

EXPERIMENTAL SETUP AND MEASUREMENTS

The experimental dataset relied upon herein for validation purposes has been obtained by Volkov and Strizhak [5]. The experimental configuration consists of a single water droplet (with a diameter between 2.67 and 3.37 mm) suspended in a hollow and transparent silica-glass cylinder of 0.1 m inner diameter. A hot air blower positioned below the cylinder blows hot air upwards with temperatures between 100 and 800°C and velocities between 3 and 4.5 m/s. The air temperatures are measured with a fast chromel-alumel (type K) thermocouple and the air velocity is controlled with the PIV technique. The time history of the droplet temperature field is obtained using the PLIF (Planar Laser-Induced Fluorescence) technique. At the moment of droplet placement on the symmetry axis of the glass cylinder, there exists already a temperature difference between the surface and the inside of the droplet, because the hot air flow is generated before the droplet placement. From a modelling perspective, since a uniform droplet temperature is assumed, an average of the initial temperature field is estimated based on the information provided in [5]. For the cases where such information is not available in [5], a default value of 30°C is taken. CCD images of the droplet are analysed during the heating process in order to monitor the time evolution of its radius until its complete evaporation, i.e., over the full droplet lifetime, \( t_d \). It is stated in [5] that the material of the holder by which the water droplet is suspended does have an influence on the conditions of heating and thus \( t_d \). In [5], the water droplet is held by a hollow metal rod. Nevertheless, two other types of material have been tested with a higher and a lower thermal conductivity. The hollow metal rod provided the medium droplet lifetime. The difference in the droplet lifetimes did not exceed 15%. Based on this, the experimental uncertainty considered herein is set to be 8% (given that the metal rod has an intermediate thermal conductivity). The test conditions and the results in terms of \( t_d \) and droplet saturation temperature, \( T_{d,sat} \), are displayed in Table 1.

RESULTS

First, simulations are carried out using Eq.(1) and \( K_1 = K_2 = 0.6 \). This is referred to hereafter as the ‘standard’ Ranz-Marshall (R&M) model. A second series of simulations is carried out with modified values of \( K_1 \) and \( K_2 \), which is referred to as the modified R&M model.

Standard R&M model

Figure 1a shows an overall good agreement between the predicted and the measured droplet lifetimes. In fact, based on the methodology proposed in [8] for the quantification of the predictive uncertainty of complex models, the overall model uncertainty (over the full range [100 – 800°C] of air temperatures tested) is about 34% with a bias factor of about 1.13. Furthermore, one can clearly visualize in Fig.1a that the agreement is even better (with a model uncertainty of 5%) if the results for the low air temperatures, and more specifically 100 and 200 °C, are discarded. These results are quite surprising, because the initial range of applicability of the R&M model is up to 200°C and it is very often reported in the literature (e.g., [3]) that a large temperature gradient between the droplet and the ambient air leads to a significant mass transfer reduction, which is generally accounted for by modelling a reduction factor for the Sherwood number. Some of the proposed
correlations have been reviewed in [2-3]. Based on the current results, this was not necessary for the case at hand although expressions (1) (with $K_1 = K_2 = 0.6$) were used beyond their initial range of validity in terms of free stream air temperature.

Table 1. Experimental data [5].

| $T_a$ (°C) | $U_a$ (m/s) | $d_{d,0}$ (mm) | $T_{d,0}$ (°C)$^a$ | $t_d$ (s) | $T_{d,sat}$ (°C)$^b$ |
|------------|-------------|----------------|-------------------|----------|---------------------|
| 100        | 3.0         | 2.67           | 30                | 87.2     | 40 ± 10             |
| 100        | 3.0         | 3.06           | 10                | 108.0    | 25 ± 10             |
| 200        | 3.0         | 3.37           | (30)              | 145.0    | -                   |
| 200        | 3.0         | 2.67           | (30)              | 61.8     | -                   |
| 200        | 3.0         | 3.06           | 35                | 74.9     | 40 ± 10             |
| 200        | 3.0         | 3.37           | (30)              | 101.7    | -                   |
| 200        | 4.0         | 3.06           | (30)              | 60.6     | -                   |
| 200        | 4.5         | 3.06           | (30)              | 56.4     | -                   |
| 300        | 3.0         | 2.67           | 25                | 49.1     | 40 ± 10             |
| 300        | 3.0         | 3.06           | 25                | 54.8     | 40 ± 10             |
| 300        | 3.0         | 3.37           | (30)              | 76.0     | -                   |
| 400        | 3.0         | 2.67           | (30)              | 33.0     | -                   |
| 400        | 3.0         | 3.06           | 35                | 37.4     | 45 ± 10             |
| 400        | 3.0         | 3.37           | (30)              | 49.7     | -                   |
| 400        | 4.0         | 3.06           | (30)              | 32.1     | -                   |
| 400        | 4.5         | 3.06           | (30)              | 30.2     | -                   |
| 500        | 3.0         | 2.67           | 30                | 23.7     | 50 ± 10             |
| 500        | 3.0         | 3.06           | (30)              | 26.6     | -                   |
| 500        | 3.0         | 3.37           | (30)              | 38.7     | -                   |
| 550        | 3.0         | 3.06           | (30)              | 24.7     | -                   |
| 600        | 3.0         | 2.67           | 35                | 17.8     | 50 ± 10             |
| 600        | 3.0         | 3.06           | 35                | 22.8     | 50 ± 10             |
| 600        | 3.0         | 3.37           | (30)              | 31.8     | -                   |
| 600        | 4.0         | 3.06           | (30)              | 20.3     | -                   |
| 600        | 4.5         | 3.06           | (30)              | 19.4     | -                   |
| 650        | 3.0         | 2.67           | (30)              | 14.6     | -                   |
| 650        | 3.0         | 3.06           | (30)              | 19.7     | -                   |
| 650        | 3.0         | 3.37           | (30)              | 26.7     | -                   |
| 700        | 3.0         | 2.67           | (30)              | 12.5     | -                   |
| 700        | 3.0         | 3.06           | (30)              | 16.5     | -                   |
| 700        | 3.0         | 3.37           | (30)              | 19.7     | -                   |
| 750        | 3.0         | 2.67           | 40                | 10.6     | 60 ± 10             |
| 750        | 3.0         | 3.06           | 40                | 14.4     | 50 ± 10             |
| 750        | 3.0         | 3.37           | (30)              | 15.9     | -                   |
| 790        | 4.0         | 3.06           | (30)              | 12.7     | -                   |
| 790        | 4.5         | 3.06           | (30)              | 12.4     | -                   |

$^a$These are estimates based on the profiles provides in [5]. A default value of 30°C (values between brackets) is assigned for cases where the information is not provided in [5].

$^b$These are estimates based on the profiles provided in [5].

Regarding the droplet saturation temperature, there is, unfortunately, not enough data reported in [5] to undertake a statistical analysis similar to the droplet lifetimes, using the methodology developed in [8]. Nevertheless, the results reported in Fig.1b clearly show that the predicted saturation temperatures are generally higher than the measured values. Furthermore, the deviations are more substantial for the highest air stream temperatures. For example, when the air temperature is around 800°C, the estimated droplet saturation temperature is around 60 ± 10°C, whereas the predicted value is 85°C. This first series of simulations has shown that, when the standard R&M model is used, the droplet lifetimes are overpredicted for low air temperatures (100 and 200°C). This suggests an underestimation of the mass
transfer coefficient (and thus, the Sherwood number) in these cases. This is qualitatively in line with the experimental findings reported in [9] where the heat and mass transfer processes have been found to be significantly more pronounced than what is suggested by the standard R&M model, although the range of conditions examined therein (i.e., air temperature range of 23-200°C, air velocities from 0.25 to 1.00 m/s and droplet Reynolds numbers from ~30 to 100 [9]) is within the range of the applicability of the R&M model proposed in [1]. In terms of droplet saturation temperature, deviations are more pronounced for high air temperatures, which might suggest an overestimation of the heat transfer coefficient and thus, the Nusselt number.

Fig. 1. Comparison between the predicted (with the standard and modified R&M model) and measured values of the droplet (a) lifetime and (b) saturation temperature.

**Modified R&M model**

In this paper, instead of examining the myriad of correlations proposed in the literature (see [2-3]), we have chosen to perform a sensitivity analysis on $K_1$ and $K_2$ (an alternative could have been an inverse modeling procedure) and remain consistent with the theoretical requirement of $Nu = 2$ and $Sh = 2$ at $Re_d = 0$. The purpose is not to propose a new correlation, but rather discuss the significance of the values in Table 2 that have been found to give a very good agreement for both the droplet lifetime and saturation temperature.

| Air temperature (°C) | $K_1$ | $K_2$ |
|----------------------|-------|-------|
| 100                  | 1.8   | 1.8   |
| 200                  | 2.0   | 0.8   |
| 300                  | 1.8   | 0.6   |
| [400 – 650]          | 3.0   | 0.6   |
| [700 – 790]          | 4.0   | 0.6   |

The improvement in the results is shown in Fig. 1, where a better agreement is obtained for the droplet lifetimes, including cases with air temperatures of 100 and 200°C (see Fig.1a). The overall model uncertainty, in this regard, has been reduced from 34% in the standard R&M model to 5% in the modified model. Furthermore, Fig.1b shows a clearly better agreement for the droplet saturation temperatures. Displaying these improved results is, per se, not the main goal of the paper. What is more interesting to discuss is the selection procedure of the coefficients $K_1$ and $K_2$. For $T_a = 100°C$, the high value of $K_1 = 1.8$ in comparison to the standard value of 0.6 can be easily explained by the need to increase mass transfer in order to reduce the overpredicted droplet lifetimes with the standard R&M model. However, for the same case, the need to substantially increase $K_2$ to 1.8 is not obvious. In fact, when only $K_1$ (and thus $Sh$) is increased, the coefficient $\alpha_2$ (in Eq.(5)) increases and leads to a significant reduction in heat transfer due to evaporation-induced cooling (see Eq.(4)). The reduced droplet temperature results in a reduced concentration of water vapor at the droplet surface (by virtue of the Clausius-Clapeyron equation) and thus, a reduced driving force for evaporation. Consequently, the droplet lifetimes remain overestimated. Therefore, in the case of $T_a = 100°C$, to keep the influence of an increased $K_1$, the value of $K_2$ had to be increased simultaneously, maintaining the evaporation-
induced cooling (see Eq.(4)) to the same level as for the case $Sh = Nu$. For the other end of air temperature range, i.e., $T_a$ between 700 and 790°C, there is a different dynamics in the heat and mass transfer coupling. Based on the initial results with the standard R&M model, one would think that since the droplet lifetimes are well predicted and the droplet saturation temperatures are not, only the Nusselt number, and thus $K_2$, should be reduced and $K_1$ could be kept equal to 0.6. This ‘optimization’ strategy was not fruitful because a reduction in Nu yielded a strong reduction in the droplet temperature (see Eqs.(5) and (4)) and thus the droplet evaporation rate (the droplet lifetimes were then overestimated). However, by keeping $K_2 = 0.6$ and increasing the value of $K_1$ to 4, the evaporation-induced cooling was increased so that the droplet saturation temperatures are reduced to values that are closer to the experimental estimates. An increase of $K_1$ to 4 did not deteriorate the good predictions of the droplet lifetimes with the standard R&M model because at high temperatures the droplet Reynolds numbers are reduced (due to the reduced gas density). Thus, the influence of $K_1$ on the Sh is reduced. Consequently, the evaporation rates do not change substantially. The choice of the $K_1$ and $K_2$ values for the intermediate air temperatures between 100 and 790°C was based on a trade-off between the two selection strategies explained above (for the two bounds of the air temperature range).

**CONCLUSIONS**

In this paper we investigated the influence of the modelling for the Sherwood and Nusselt numbers on the heating and evaporation of water droplets. To this purpose, we developed an in-house code based on the ‘film theory’ concept that is typically used in Computational Fluid Dynamics (CFD). The assessment of the modelling and the analysis of the results is based on the experiments carried out in [5]. The results show that the standard values proposed in [1] give rather poor predictions for the droplet lifetimes when the air temperature is 100 or 200°C, but surprisingly good predictions for higher air temperatures. However, at high air temperatures, the droplet saturation temperatures are overestimated. A detailed analysis of the effect of the constants $K_1$ and $K_2$ on the accuracy of the predictions shows that they should be only equated for $T_a = 100°C$ but with a higher value of 1.8. For higher air temperatures, a high value of $K_1$ promotes evaporation-induced cooling (and thus, reduced droplet saturation temperatures) without significantly affecting evaporation rates (and thus, the droplet lifetimes). In the light of the present results, the ‘classical’ Ranz-Marshall approach with $K_1 = K_2 = 0.6$ is clearly not optimal. A more thorough analysis, with eventually additional experimental data, is required.

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