Assessment of the Fire Dynamics Simulator Modeling for the Heating and Evaporation of a Single Water Droplet at Moderate and High Temperatures

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ABSTRACT

The work described in this paper is undertaken with the purpose of providing a detailed assessment of the current modelling capabilities of the effects of fire suppression systems (e.g., sprinklers) in fire-driven flows. Such assessment will allow identifying key modelling issues and, ultimately, improving the reliability of the numerical tools in fire safety design studies. More specifically, we studied herein the heating and evaporation of a single water droplet. This rather ‘simple’ configuration represents the first step in a tedious and rigorous verification and validation process, as advocated in the MaCFP (Measurement and Computation of Fire Phenomena) working group (see https://iafss.org/macfp/). Such process starts ideally with single-physics ‘unit tests’ and then more elaborate benchmark cases and sub-systems, before addressing ‘real-life’ application tests. In this paper, we are considering the recently published comprehensive and well-documented experimental data of Volkov and Strizhak (Applied Thermal Engineering, 2017) 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 high temperatures considered therein represent a strong element of novelty, since previous experimental studies on single droplets were limited to rather relatively ‘moderate’ temperatures, up to around 350°C. Furthermore, the monitoring of the time history of the droplet temperature field, in addition to the droplet lifetime, provides very useful information for model development and validation purposes. In this numerical study, 36 experimental tests have been simulated with the Fire Dynamics Simulator (FDS 6.6.0). The results show that the droplet lifetime is overpredicted with an overall accuracy of 31%. The accuracy in the range 300 to 800°C is even better, i.e., 7 %, whilst the cases of 200 and, more so 100°C, showed much stronger deviations. The measured droplet saturation temperatures did not exceed 70°C, even for high air temperatures of around 800°C, whereas the predicted values approached 100°C. Based on the current findings, further analysis is required on the modelling of the heat and mass transfer coefficients, and more specifically the sub-models for the Nusselt and Sherwood numbers.

KEYWORDS: modeling; suppression; sprinklers; evaporation; Fire Dynamics Simulator.
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. In most of the Computational Fluid Dynamics (CFD) codes, droplet evaporation modelling is based on the so-called ‘film theory’ [1]. The film is a very thin layer at the interface between the liquid and the surrounding environment where heat and mass exchange as well as phase transformation occur. The thickness of the film is generally significantly (sometimes orders of magnitude) smaller than typical cell sizes used in fire dynamics (or combustion) simulations, except if Direct Numerical Simulations (DNS) are carried out, which could not be afforded for practical fire scenarios. Consequently, several correlations have been developed in the literature to estimate the convective heat and mass transfer film coefficients around droplets. These correlations are based on single suspended water droplet experiments where the droplet is subjected to a convective air flow (natural or forced) with a fixed velocity and temperature. The most widely used correlations date back to the early work of Ranz and Marshall for a forced convection flow [2] where the evaporation of water droplets in air is examined for a room temperature up to 220°C, a droplet diameter between 0.6 and 1.1 mm and a droplet Reynolds number, Re_d, between 2 to 200. Thanks to the significant advances in measuring technologies that could be used to characterize in detail the heating and evaporation process of a water droplet, more accurate data is available for model validation. For example, very recently, Volkov and Strizhak [3] published a very interesting set of data for the heating and evaporation of a water droplet with a diameter between 2.6 and 3.4 mm in a hot environment with free stream temperatures between 100 and 800°C and velocities between 3 and 4.5 m/s. The objective of this paper is to rely on this dataset to assess the capabilities of a CFD code, namely the Fire Dynamics Simulator (FDS 6.6.0), in the modelling of the heat up and evaporation process of single suspended water droplets [4-6].

NUMERICAL MODELLING
A detailed description of the mathematical modelling for droplet evaporation in FDS 6.6.0 is provided in [4-6]. Only the main equations for the case at hand are recalled herein for the sake of clarity. The mass and energy conservation equations for a single spherical liquid droplet (in the absence of interaction with solid boundaries) read [4-5]:

\[
\frac{dm_d}{dt} = A_d \frac{Sh D_g}{d_d} \rho (Y_v - Y_l)
\]

\[
\frac{m_g c_p}{dt} = A_d \frac{Nu k}{d_d} (T_g - T_f) + \frac{dm_d}{dt} L_v + q_r
\]

where \(m_d, A_d, d_d\) and \(T_f\) are respectively the mass, area, diameter and temperature of the droplet, \(c_p\) and \(L_v\) are the specific heat and latent heat of vaporization of water, \(\rho, k\) and \(T_g\) are respectively the density, thermal conductivity and temperature of the surrounding gas, \(q_r\) is a radiative source term, \(D_g\) is the binary diffusion of water vapor in the surrounding gas (i.e., air), \(t\) is the time and \(Y_v\) and \(Y_l\) are the mass fraction of water vapor at the droplet surface and in the surrounding gas, respectively. The Sherwood, \(Sh\), and the Nusselt, \(Nu\), numbers are expressed as [2]:

\[Sh = 2.0 + 0.6 Re_d^{1/3} Sc^{1/3}\quad \text{and}\quad Nu = 2.0 + 0.6 Re_d^{1/3} Pr^{1/3}\]

where \(Re_d\) is the droplet Reynolds number, \(Sc\) and \(Pr\) are respectively the Schmidt and the Prandtl numbers, taken as \(Sc = 0.6\) and \(Pr = 0.7\) (see page 87 in [6]). The droplet Reynolds number, \(Re_d\), is calculated as:

\[
Re_d = \frac{d_d |u_d - u_g| \rho}{\mu(T_{film})}
\]

where \(u_d\) and \(u_g\) are respectively the droplet and gas velocity vectors and \(\mu(T_{film})\) is dynamic viscosity of air at the film temperature, \(T_{film}\), which is calculated using the one-third rule.

Equations (1) and (2), which are coupled to the equations for the gas temperature and the rate of change of vapor mass in the gas, are solved semi-implicitly over the course of a gas phase time step [5].
EXPERIMENTAL SETUP AND COMPUTATIONAL TESTS

Experimental setup and measurements

The experimental dataset relied upon herein for validation purposes has been obtained by Volkov and Strizhak [3]. 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.

Table 1. Experimental data [3].

| $T_a$ (°C) | $U_a$ (m/s) | $d_{d,0}$ (mm) | $T_{d,0}$ (°C)$^a$ | $t_l$ (s) | $T_{sat}$ (°C)$^a$ |
|------------|-------------|----------------|-------------------|---------|------------------|
| 100        | 3.0         | 2.67           | 30                | 87.2    | 40 ± 10          |
| 100        | 3.0         | 3.06           | 10                | 108.0   | 25 ± 10          |
| 100        | 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    | -                |
| 790        | 3.0         | 2.67           | 40                | 10.6    | 60 ± 10          |
| 790        | 3.0         | 3.06           | 40                | 14.4    | 50 ± 10          |
| 790        | 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 provided in [3]. A default value of 30°C (values between brackets) is assigned for cases where the information is not provided in [3].

$^b$These are estimates based on the profiles provided in [3].
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 [3]. For the cases where such information is not available in [3], 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 [3] 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 [3], 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, \( T_{d,\text{sat}} \) are displayed in Table 1.

### Computational tests

The setup of the computational tests described in Table 1 is similar to the verification test case water_evaporation_5\(^1\) described in [4] where stratification and noise (in the flow field) are turned off and the ambient pressure and temperature are fixed. For the case at hand, \( p_{\text{amb}} = 101325 \) Pa and \( T_a \) is fixed based on the values displayed in Table 1. Note also that the default radiation settings are turned on in this paper (as opposed to water_evaporation_5), given the relatively high gas temperatures that are involved. For example, at 790°C and without radiation the droplet lifetime increased by around 60% and the droplet saturation temperature decreased by about 10°C. An additional aspect that has been considered for the tests carried out herein and not for the test case water_evaporation_5 is the setup of a uniform velocity field using specific options available in FDS and which allow ‘forcing’ the gas velocity field within the computational domain and ‘freezing’ that field throughout the calculation [6]. In other words, the flow field is not solved but imposed. Additional calculations that took into account turbulent fluctuations (by setting a velocity ‘noise’ of up to 20%) showed that the results varied by less than 1%.

### RESULTS

Figure 1a shows an overall good agreement between the predicted and the measured droplet lifetimes. In fact, based on the methodology proposed in [7] 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 31% with a bias factor of about 1.71. Furthermore, one can clearly visualize in Fig.1a that the agreement is even better if the results for the low air temperatures are discarded. This is quantified in Table 2 which indicates that the model uncertainty reduces to 15% for the range [200 – 800°C] and 7% for the range [300 – 800°C].

![Fig. 1. Comparison between the predicted and measured values of the droplet (a) lifetime and (b) saturation temperature.](https://github.com/firemodels/fds/blob/master/Verification/Sprinklers_and_Sprays/water_evaporation_5.fds)
These results are quite surprising, because it is very often reported in the literature (e.g., in [8]) 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. Based on the current results, this was not necessary for the case at hand although expressions (3) were used beyond their initial range of validity.

Table 2. Bias factor and model relative standard deviation depending on the air temperature range.

| Air temperature (°C) | [100 – 800] | [200 – 800] | [300 – 800] |
|----------------------|-------------|-------------|-------------|
| Bias factor, δ       | 1.71        | 1.61        | 1.57        |
| Relative standard deviation, ωM | 0.31 | 0.15 | 0.07 |

For the cases of \( T_a = 200°C \), and even more so for \( T_a = 100°C \), the droplet lifetimes are significantly overestimated, indicating an underestimation of the mass transfer process. This aspect has been discussed in [9] where an alternative to Eqs. (3) has been proposed, based on single droplet drying experiments over an air temperature range of 23-200°C and with \( Re_d \) from 30 to 100. The expression proposed in [9] for heat transfer reads:

\[
Nu = 6.4 + 0.8Re_d^{1/2}Pr^{0.1}
\]  

(5)

The significantly higher value of 6.4 for the natural convection regime (and obtained after extrapolation), in comparison to the theoretical value of 2, is attributed in [9] to (1) a thermal gradient within the medium surrounding the droplet and which is induced by molecular diffusion, and (2) localized convection currents that increase heat and mass transfer. Equation (5) and other alternatives to Eqs.(3) need thus be implemented and tested against the experimental data used herein.

Regarding the droplet saturation temperature, there is, unfortunately, not enough data reported in [3] to undertake a statistical analysis similar to the droplet lifetimes, using the methodology developed in [7]. However, the results reported in Fig.1b and Fig.2 clearly show that the predicted saturation temperatures are generally higher than the measured values. This is particularly the case when the air temperature is high, as shown in Fig.2b where the measured droplet saturation temperatures did not exceed 60°C whereas the predicted values approached 100°C. This demonstrates the need to undertake a detailed analysis on the coupled processes of heat and mass transfer around the droplets in order to achieve a good agreement for the droplet lifetime and saturation temperature simultaneously. Furthermore, the present results may imply that the problems of potential numerical instability and super-saturation that have been addressed in [4] can be due (in some cases) to the physical model of heat transfer around the droplet, and which makes the droplet reach a too high saturation temperature.

Fig. 2. Comparison between the time-evolution profiles of the measured temperature on the surface and inside the droplet and the predicted droplet temperature for \( d_{d,0} = 3.06 \) mm, at \( U_a = 3 \) m/s and at different air temperatures. (a) \( T_a = 200°C \). (b) \( T_a = 790°C \).
CONCLUSIONS

In this paper we assessed the capabilities of the Fire Dynamics Simulator (FDS 6.6.0) in the modelling of the heat up and evaporation of a water droplets based on the experiments carried out by Volkov and Strizhak (Applied Thermal Engineering, 2017). In these experiments, 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, based on the simulation of 36 tests, show that the droplet lifetime is predicted with an overall accuracy of 31%. The accuracy in the range 300 to 800°C is even better, i.e., 7 %, whilst the cases of 200 and, more so 100°C, showed much stronger deviations that indicate an underestimation in the mass transfer rate for these moderate temperatures. Furthermore, the measured droplet saturation temperatures did not exceed 70°C, even for high air temperatures of around 800°C, whereas the predicted values approached 100°C. Thus, based on the current findings, further analysis is required on the modelling of the heat and mass transfer coefficients, and more specifically the sub-models for the Nusselt and the Sherwood numbers.

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