Development of a novel two-zone model for the heating of an evaporating liquid droplet

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Highlights:

- A novel two-zone model for the heating of an evaporative droplet is implemented.
- The two-zone model is compared to the isothermal model.
- Similar predictions for the lifetimes and saturation temperatures are found.
- Evaporative cooling is more pronounced at the early stages with the two-zone model.

Abstract:

A novel two-zone model is implemented, within an in-house code, for the heating of an evaporating droplet. While it is not yet possible to fully assess and validate the novel model due to lack of available detailed experimental data, the concept is described. Differences compared to the ‘common’ isothermal model are explained. Firstly, a quantitative assessment is performed, using experimental datasets where a suspended water droplet is exposed to a hot air flow. Secondly, the behavior of the novel model is examined over a wider range of conditions in terms of air velocity, ambient temperature and initial droplet diameter.

The novel model predicts droplet lifetimes and saturation temperatures that are similar to the isothermal model. Nevertheless, the results also show that, during the early stages, the cooling of the surrounding gas due to the evaporation of the droplet is more pronounced with the two-zone model. During a second stage, the evaporation term is slightly lower than with the isothermal model. The available data do not allow to fully assess which result is closer to reality, but the important observation is that there exist differences. These differences increase with higher ambient temperature, relative velocity or initial diameter.

Keywords: evaporation; modelling; two-zone; liquid droplet; suppression

1. Introduction

Accurate modelling of droplet heating and evaporation is highly relevant in the field of fire safety. Many active fire protection systems, such as sprinklers and water mist, involve the heating and evaporation of water droplets as they interact with smoke and flames [1, 2, 3]. Several heating and evaporation models have been developed in the literature since the reference work of Abramzon and Sirignano [4]. Several types of models are summarized in this introduction, based on [5] and [6].

The simplest model is the isothermal model – a.k.a. infinite thermal conductivity (ITC) model – which implies a uniform temperature field inside the droplet. Although this model is a strong simplification of reality, it is widely used in Computational Fluid Dynamics (CFD) packages,

e.g., the Fire Dynamics Simulator (FDS) [7] due to its simplicity and the subsequent low computational cost. At the other end of the spectrum (in terms of model complexity), the most advanced approach is to solve the full set of Navier-Stokes equations inside the droplet. This provides more insight onto the physics and may contribute to the development of simplified models for engineering purposes. Nevertheless, it is not a viable approach for practical applications involving complex flow fields and millions of droplets. Hence models of intermediate complexity have been developed, such as the thermally thick approach in FDS, i.e. a 1D heat transfer by conduction model [7]. Then many other models of intermediate complexity are based on a ‘prescribed’ shape of the temperature profile inside the droplet. A comprehensive review of these models is provided in [8]. The variety of these models (e.g., parabolic model [9], power law model [10], polynomial model [11] and heat balance integral method [12]) stems essentially from the nature of the functional form that is used for the temperature distribution. In the parabolic approximation, a quasi-steady profile is immediately assumed, without transient stage [8]. This is improved in the power law method proposed by Bereton [10] by adjusting dynamically the power law dependence at the early stages of the heating process until steady state is reached and the model switches to the parabolic profile. The polynomial approximation method is a combination of the two latter methods. A more accurate treatment of droplet heating is provided by the heat balance integral method which captures better the transient behavior. The methodology consists of dividing the droplet in two concentric zones, an inner cold layer (which always remains at the initial temperature level) and an outer hot layer (also called thermal layer) where the temperature profile is assumed to be parabolic. The thickness of the thermal layer increases with time. It should be noted that, regardless of the functional form for the temperature profile, there are two options for the thermal conductivity of the liquid. The first option is to use the ‘actual’ (real) conductivity. The second option is to use an ‘effective’ thermal conductivity coefficient, which is higher than the actual one. The purpose is to account (indirectly) for the increased heat transfer within the liquid, which is induced by internal recirculation under the effect of shear stresses at the surface.

Despite the variety of alternative models, the isothermal model remains the most ‘popular’ in the combustion and fire science and engineering fields. This is partly due to the lack of detailed experimental data that would greatly help providing compelling evidence as to the added value (or not) of more advanced models (than the isothermal one) in terms of accuracy, bearing in mind the potential increase in computational cost. The development of new measurement techniques in the recent years offers the possibility to revisit the models and, eventually, develop new ones. An example of new available experimental datasets is presented in [13, 14] where the Planar Laser Induced Fluorescence (PLIF) technique is used to provide detailed temperature distributions inside a single suspended water droplet subjected to a convective hot air flow. An additional element of novelty in the dataset is that the ambient hot air temperature reached up to 790°C, whereas most of the previously available data was limited to moderate temperatures of about 300 to 400°C. The temperature distributions displayed in [13, 14] are strongly inhomogeneous, especially in the early stages of heating and evaporation. These stages can be highly important in practical applications, knowing for example that the travel time of a water droplet from a sprinkler or a water mist nozzle to the floor level is (at most) in the order of few seconds. On the other hand, it is mentioned in [8] that in single-suspended droplet experiments, the effect of the temperature inhomogeneity on the prediction of droplet lifetimes (time to complete evaporation) is rather marginal.

In [15] the effect of the sub-models for the Sherwood and the Nusselt numbers and the possible modifications to those sub-models to have a better agreement between simulations with the isothermal model and the experimental results obtained by Volkov and Strizhak was investigated. The effort in [15] was put on the saturation temperature and the droplet lifetime. However, in the present paper, the focus is put on the investigation of the thermal gradient inside the droplet through the implementation of a novel model (i.e. the two-zone model) without changing the ‘standard’ models for the Sherwood and the Nusselt numbers. The two papers hence investigate different aspects. At a more developed stage, the effects could be coupled.

The novel model is proposed based on the overall framework of the heat balance integral method. The key novelties are that: (i) the inner zone does not remain cold, and (ii) the temperature is uniform within each zone. The novel model is believed to be simpler to implement than the ones described above, while it will be illustrated that there are differences with the isothermal model. Moreover, the novel model has the potential to capture non-uniformity of temperature in the droplet with limited computational cost. In the remainder of the paper, the main assumptions and equations of the proposed two-zone model are explained before assessing the results against the experimental dataset of [13, 14]. The in-house code results are also assessed against FDS results obtained using the available spherically symmetrical solver for heat transfer inside the droplet [7]. Then the behavior of the model is explored over a wider range of conditions. For instance, higher convective heat flow velocities are considered, corresponding in practical configurations to higher droplets Reynolds number (typically closer to the nozzle). The behavior of the model is systematically analyzed and compared against the outcome of the ‘common’ isothermal model.

2. Numerical Modeling

The main equations for heat and mass transfer are described in this section. The evaporation rate is calculated using the classical ‘film theory’. The novelty lies in the two-zone treatment of heat transfer (subsection 2.2).

2.1 Mass transfer

The evaporation rate of a spherical droplet, using the ‘film theory’ and taking into account the Stefan-flux, could be expressed as [3]:

$$\frac{d m_d}{dt} = \dot{m}_d = - \pi d_d Sh \frac{k_{Film}}{Le c_{p,v,Film}} \ln(1 + B_M) \quad (1)$$

where m_d and d_d are, respectively, the mass and the diameter of the droplet, t is the time, k_{Film} and $c_{p,v,Film}$ are respectively the thermal conductivity and the specific heat of the film. Due to space limitation, it can only be said that the 1/3 rule is used for the film properties as done in [16], while the properties of the gas and the liquid are calculated according to [17, 18, 19, 20]. In this equation, Le is the Lewis number (taken here as unity), Sh is the Sherwood number (calculated using the classical Ranz-Marshall expression [21]) and B_M is the Spalding number (as defined in [3]). The molar fraction of the vapor at the droplet surface used in the definition of the Spalding number is computed through the well-known Clausius-Clapeyron equation.

2.2 Heat transfer

Equation (1) is valid regardless of the heating model that is used. In the isothermal model, the droplet surface temperature equals the overall droplet temperature. This model implies that the heating process occurs over the entire droplet since the early stages; whereas, in reality, only a fraction of the droplet will heat up. As a consequence, the droplet surface heats up at a slower pace than reality in the isothermal model, with a direct consequence on the evaporation process, i.e., lower evaporation rates. Besides, in the isothermal approach, the droplet is expected to absorb more energy in the early stages than in reality because the rate of heat transfer by conduction is not limited by the value of the thermal conductivity (i.e., infinite thermal conductivity concept). The lower evaporation rates in conjunction with more heat absorption by the droplet can lead to significant deviations in the evaporative cooling and, more generally, the overall heat balance of the droplet. The novel model aims at improving the accuracy of the modelling without significantly increasing the computational cost.

2.2.1 The two-zone concept

The droplet is divided into two concentric zones, i.e., an outer layer and an inner layer (see Fig. 1). In each zone the temperature is assumed uniform, similarly to the two-zone concept for thermal stratification of smoke in the early stages of an enclosure fire. A uniform temperature within each zone implies an infinite thermal conductivity in each of the two layers. Yet, there is a temperature difference that drives the heat transfer process between the two zones. Thus, heat transfer within the droplet is not limited by the thermal conductivity but by the depth of the outer layer. This approach is similar to the heat balance integral method [8]. However, it is simpler because of the ‘imposed’ two-step temperature profile that is easier to solve.

Fig. 1. A schematic representation of a droplet using a two-zone approach

Based on the description provided above, the heat transfer equations for the outer (Eq. (2)) and inner layer (Eq. (3)) (without considering thermal radiation) read:

$$m_o c_{p,L} \frac{dT_o}{dt} = \dot{q}_{conv} + \dot{q}_{evap} + \dot{q}_{o-i} \quad (2)$$

$$m_i c_{p,L} \frac{dT_i}{dt} = -\dot{q}_{o-i} \quad (3)$$

where m is the mass of the layer, $c_{p,L}$ is the specific heat capacity of the liquid, T is the temperature, $\dot{q}_{conv}$ is the convective heat transfer rate at the droplet surface, $\dot{q}_{evap}$ is the evaporative cooling rate, and $\dot{q}_{o-i}$ is the heat exchange rate between the outer and the inner layers. The subscripts ‘o’ and ‘i’ refer respectively to the outer and the inner layers.

The expressions for the mass of the outer and the inner layers read:

$$m_o = \rho_L \frac{\pi}{6} d_d^3 \left[1 - \left(1 - \frac{2\delta_o}{d_d} \right)^3 \right] \quad (4)$$

$$m_i = \rho_L \frac{\pi}{6} (d_d - 2\delta_o)^3 \quad (5)$$

where δ_o is the depth of the outer layer.

The convective heat transfer rate is expressed as:

$$\dot{q}_{conv} = A_d h (T_g - T_o) \quad (6)$$

The convection coefficient is computed from the Nusselt number, which is also calculated using the classical Ranz-Marshall expression [21].

Moreover, evaporative cooling is expressed as:

$$\dot{q}_{evap} = \dot{m}_d L_v \quad (7)$$

At this stage, two key parameters remain to be modelled, namely the heat exchange rate between the two zones and the depth of the outer layer.

2.2.2 Heat exchange rate between the two zones

The heat exchange between the zones is assumed to occur at the interface (between the two zones) across the surface area, A_i , of the inner layer where ‘hot’ liquid is mixed with ‘cold’ liquid with a characteristic velocity u_m . The heat exchange rate could thus be expressed as:

$$\dot{q}_{o-i} = u_m A_i \rho_L c_{p,L} (T_o - T_i) \quad (8)$$

The choice is made here to approximate the characteristic velocity by the regression velocity at the surface (due to evaporation), i.e., $u_m = u_d = \dot{m}_d / (\rho_L A_d)$. Equation (8) can then be written as:

$$\dot{q}_{o-i} = \dot{m}_d \frac{A_i}{A_d} c_{p,L} (T_o - T_i) \quad (9)$$

2.2.3 Depth of the outer layer

The depth of the outer layer can be approximated by defining a critical Biot number of the droplet. The Biot number is the ratio of the internal thermal resistance to the external thermal resistance and gives thus information on the temperature gradient inside the droplet. It is calculated as:

$$Bi = \frac{h (d_d/2)}{k_L} \quad (10)$$

where k_L is the thermal conductivity of the liquid.

It is commonly assumed that if $Bi < 0.1$, the temperature gradient is very small, which corresponds to a thermally thin behaviour. Based on this reasoning, the depth of the thermal layer can be defined as the length scale that corresponds to the critical Biot number of 0.1:

$$\delta_o = \frac{0.1 k_L}{h} \quad (11)$$

This is in line with the assumption of infinite thermal conductivity within the outer layer, as explained previously. If the calculated depth of the outer layer is greater than (or equal to) the radius of the droplet, the model becomes the isothermal model. A sensitivity analysis on the effect of the critical Biot number, taken initially as $Bi_{crit} = 0.1$, is performed below. Moreover, if the relative temperature difference between the two layers becomes smaller than 0.1%, the two-zone model switches to the isothermal model.

3. Experimental and numerical tests

3.1 Experimental setup and measurement techniques

Table 1. List of the simulation tests with their input parameters and some results (i.e., the droplet lifetime and the saturation temperature) for the in-house codes.

Test		Initial conditions							Results			
Name	#	Gas		Droplet					Isothermal		Two-zone	
		T_g [°C]	u_g [m/s]	$d_{d,0}$ [mm]	$T_{d,0}$ [°C]	$T_{i,0}$ [°C]	$T_{o,0}$ [°C]	Bi_{crit} [-]	t_d [s]	T_{sat} [°C]	t_d [s]	T_{sat} [°C]
Reference	1	100	3	3.06	20.0	20.0	20.0	0.10	280.6	39.0	280.3	39.0
	2	300	3	3.06	20.0	20.0	20.0	0.10	71.9	65.4	71.7	65.4
	3	500	3	3.06	20.0	20.0	20.0	0.10	38.5	76.6	38.4	76.6
	4	790	3	3.06	20.0	20.0	20.0	0.10	21.7	85.3	21.6	85.3
Experiments	5	100	3	3.06	26.6	26.6	26.6	0.10	279.3	39.0	279.1	39.0
	6	300	3	3.06	30.2	30.2	30.2	0.10	71.3	65.4	70.8	65.4
	7	500	3	3.06	35.3	35.3	35.3	0.10	38.0	76.6	37.9	76.6
	8	790	3	3.06	41.6	41.6	41.6	0.10	21.3	85.3	21.2	85.3
	9	100	3	3.06	26.6	22.9	34.4	0.10	279.3	39.0	278.2	39.0
	10	300	3	3.06	30.2	27.6	38.1	0.10	71.3	65.4	70.8	65.4
	11	500	3	3.06	35.3	33.5	49.1	0.10	38.0	76.6	37.6	76.6
	12	790	3	3.06	41.6	40.8	47.6	0.10	21.3	85.3	21.1	85.3
Velocity	13	100	10	3.06	20.0	20.0	20.0	0.10	168.5	39.0	168.1	39.0
	14	300	10	3.06	20.0	20.0	20.0	0.10	43.9	65.4	43.7	65.4
	15	500	10	3.06	20.0	20.0	20.0	0.10	23.9	76.6	23.7	76.6
	16	790	10	3.06	20.0	20.0	20.0	0.10	13.7	85.3	13.5	85.3
	17	100	20	3.06	20.0	20.0	20.0	0.10	123.4	39.0	123.1	39.0
	18	300	20	3.06	20.0	20.0	20.0	0.10	32.4	65.4	32.2	65.4
	19	500	20	3.06	20.0	20.0	20.0	0.10	17.7	76.6	17.5	76.6
	20	790	20	3.06	20.0	20.0	20.0	0.10	10.2	85.3	10.1	85.3
Diameter	21	100	3	2.00	20.0	20.0	20.0	0.10	141.8	39.0	141.7	39.0
	22	300	3	2.00	20.0	20.0	20.0	0.10	36.1	65.4	36.0	65.4
	23	500	3	2.00	20.0	20.0	20.0	0.10	19.2	76.6	19.1	76.6
	24	790	3	2.00	20.0	20.0	20.0	0.10	10.8	85.3	10.7	85.3
Biot number	25	100	3	3.06	20.0	20.0	20.0	0.05	280.1	39.0	280.0	39.0
	26	300	3	3.06	20.0	20.0	20.0	0.05	71.9	65.4	71.4	65.4
	27	500	3	3.06	20.0	20.0	20.0	0.05	38.5	76.6	38.2	76.6
	28	790	3	3.06	20.0	20.0	20.0	0.05	21.7	85.3	21.5	85.3
	29	100	3	3.06	20.0	20.0	20.0	0.15	280.6	39.0	280.5	39.0
	30	300	3	3.06	20.0	20.0	20.0	0.15	71.9	65.4	71.8	65.4
	31	500	3	3.06	20.0	20.0	20.0	0.15	38.5	76.6	38.5	76.6
	32	790	3	3.06	20.0	20.0	20.0	0.15	21.7	85.3	21.7	85.3

The results of a series of experiments described in [13] and [14] are used. A single suspended water droplet with radius between 1 and 2 mm is subjected to a hot air flow with temperature (T_g) that varies from 100°C to 800°C and a velocity (u_g) that varies between 3 and 4.5 m/s. The time evolution of the droplet diameter is monitored using a CCD camera. The temperature of the droplet is measured using the PLIF method.

In the experiments, a temperature gradient is already present at the start of the experiment due to the time required to move the particle to the center of the cylinder, where the hot air is already flowing. In order to compare the numerical results to the experimental data, an initial value has to be imposed based on this initial temperature profile. Hence, in Table 1, different initial temperatures were provided for the simulations 5 to 12. Those temperatures were obtained after some post-processing of the temperature profiles provided in [13] and [14] to match with the spherical assumption made in the models.

However, as the objective of this paper is to analyze the differences and the possible improvement of the two-zone model in comparison to the isothermal model, the reference simulations (tests 1 to 4) and the simulations of the parametric study (tests 13 to 32) are run with an initial uniform temperature condition of 20°C. The influence of the initial temperature profile is analyzed using simulations 5 through 12.

3.2 Computational tests

The list of numerical simulations is displayed in Table 1. Cases 1 to 4 are used as reference. The second set of tests are chosen such that the initial conditions are representative of the experiments: in tests 5 to 8, the average initial droplet temperature is imposed in a uniform manner while in tests 9 to 12 the initial temperature gradient is approximated by imposing different temperatures for the inner and the outer layers. The remaining tests (13 to 32) provide a parametric study on the important parameters: the ambient gas temperature and velocity, the initial diameter of the droplet, the critical Biot number and the temperature dependence of the heat of vaporization.

4. Results and discussion

4.1 General trend – reference case

Regarding the saturation temperature and the droplet lifetime (Table 1), the two-zone model does not improve the predictions in comparison to the isothermal model. Similar deviations are reached with the two in-house models in comparison to the available experimental data. Nevertheless, it is argued that the early stages in the droplet heat-up and evaporation are more important, as in many applications (typically sprinkler systems) the droplets only take a few seconds to reach the floor, which may not be sufficient to fully justify the infinite conductivity model. Therefore, the focus is essentially put on the transient heating stage, i.e., the first seconds.

Figure 2 shows the time evolution of the temperature and the diameter for test 3. Similar behavior is obtained for the other simulations. While impossible with the isothermal model, a distinction can be made between the surface and the average temperatures in the two-zone concept. Figure 2 shows, as expected, that the surface temperature reaches almost saturation (around 76.6 °C) more quickly in the two-zone model (around 3 s) than in the isothermal model.

The difference in temperature predictions between the two models does not have a noticeable influence on the predicted droplet lifetime (around -0.3% of relative difference between the two approaches), which remained higher than the experimental value of 26.6 s by 44.3%. The deviation between the two models is attributed to the deviation in the early stages of the heating process (Fig 2, c). However, due to the slower increase of the inner temperature, the two-zone model displays an average temperature that is lower than in the isothermal model (not shown).

After about 32 s (not shown), the two-zone model converges to the isothermal model because the temperature difference between the two liquid zones becomes less than 0.1%. Yet, the Biot number of the droplet remains above 0.10 during almost the entire droplet lifetime (it is around 0.22 after 32 s, not shown).

Fig. 2. A zoom on the initial time evolution of (a) the surface temperature, (b) the inner temperature, (c) the diameter, and (d) the evaporation rate¹ for test 3, i.e. $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$

In Fig. 2 the simulation results are also compared to the numerical results based on a spherically symmetric heat conduction solver, using the implementation of the thermally thick droplet model in FDS (version 6.7.3) [7]. The setup of the computational tests is similar to the setup of the verification test case ‘Ranz_Marshall_thermally_thick’². The only modifications to this set-up are in the ambient conditions, in order to match the present case, and the flow field imposed, rather than solved (as done in [15]). The results mainly show that during the early stages of the heat-up and evaporation processes, the increase in surface temperature in the thermally thick model is better captured by the two-zone model than with the isothermal model. Then it can be seen that the FDS simulation provides a saturation temperature (around 73°C) that is lower than the two in-house code models. Figure 2 shows also that the inner temperature in the ‘thermally thick’ simulation is better captured by the two-zone model during the first second, i.e., no immediate temperature rise. At a later stage, the center temperature from the thermally thick model

¹ In the FDS simulation results we noticed some fluctuations that we smoothed, for the sake of clarity.

² https://github.com/firemodels/fds/blob/master/Verification/Sprinklers_and_Sprays/Ranz_Marshall_thermally_thick.fds

increases faster than the inner layer temperature. This is not as expected, given that the inner temperature in the thermally thick approach is taken as the temperature in the center of the droplet; it is not a spatially-averaged temperature. This deserves further investigations. Finally, it can be observed that the isothermal temperature overestimates the temperature field inside the droplet. Regarding the temporal evolutions of the diameter and the evaporation rate, it can be observed that during the first second, the two-zone model provides results that are closer to the thermally thick simulation.

One of the main goals of the use of water sprays in fire protection systems is to cool down the surrounding gas. The largest contribution is the heat taken by the droplet to evaporate at the surface. This can be quantified by the evaporation term, i.e., Eq. (7). Figure 3 shows the time evolutions of this term with the two-zone and the isothermal models. The relative difference, ε , is also provided on the graph:

$$\varepsilon = \frac{q_{\text{two-zone}} - q_{\text{iso}}}{q_{\text{iso}}} \quad (12)$$

The cooling effect due to the evaporation is stronger for the two-zone model than for the isothermal model during the first seconds. Even though the surface temperatures seem similar for the two models (Fig. 2, a), the difference in the evaporation rate (and thus, in the evaporative cooling) is still substantial due to the exponential function in the Clausius-Clapeyron equation. This explains the high peak value (around 70%) for the relative difference. After 4 s, this difference becomes very small (in line with Fig. 2, a), and even slightly negative because the surface temperature is slightly lower for the two-zone model (due to the impact of heat exchange term between the two layers). The relative difference evolves towards zero as the two surface temperatures converge to the saturation temperature (notwithstanding the significant deviation in the end, caused by the small denominator in Eq. (12) then).

Fig. 3. Time evolution of the evaporative cooling of the droplet on the surrounding gas and the relative difference between the two models for test 3: $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $T_{\text{init}} = 20\text{ }^{\circ}\text{C}$, $Bi_{\text{crit}} = 0.10$

4.2 Influence of the initial temperature gradient

As mentioned previously, a temperature gradient is already present in the droplet at the beginning of the experiments, see Fig. 4. As a result, the initial average temperature is higher than the 20°C chosen for the reference cases. Therefore, two extra groups of simulations are run. The first group consists of simulations where the same initial temperature, computed from the experimental profile, is imposed for the two models. For the second group, the average initial temperature imposed in the two-zone model is the same as in the isothermal model. Nevertheless, different initial temperatures are assigned to each layer. These temperatures are

computed from the experimental data using the least-square method as described in [22], but adapted to a spherical volume.

Fig. 4. Comparison of the initial temperature profile for the experimental data, the isothermal model and the two-zone model for test 7, i.e. $T_g = 500\text{ }^\circ\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $Bi_{crit} = 0.10$

The main variations in the evolution of the temperature occur during the first two seconds (see Fig. 5). As expected, the outer layer temperature computed when the initial temperature gradient is considered is higher than when only the average temperature is used as initial condition. The same comment can be made for the average temperature (not shown) while for the inner layer temperature, it is the opposite. After two seconds, the difference decreases and the results of the two simulations converge again to the same results.

Fig. 5. Comparison of the time evolution (the first 5s) of the temperature for the isothermal model (yellow), for the two-zone model without an initial temperature gradient (purple), for the two-zone with an initial temperature gradient (green), for the two-zone model with an initial temperature gradient and a value of 0.28 for the critical Biot number (grey), and the experimental data (black) for the conditions $T_g = 500\text{ }^\circ\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$

In [13, 14] the temporal evolution of the temperature is provided along several directions from the center to the surface of the droplet. From this information, an average center temperature and an average surface temperature are calculated. From the experimental data it can be seen that, at 0 s, a temperature gradient is already present in the droplet. Figure 5 also shows that both models (the two-zone model and the isothermal model) overestimate the temperature rise measured experimentally. After two seconds, the surface temperatures obtained in both models are already higher than the experimental surface temperature, similarly to the findings reported in [3]. Furthermore, it can be seen that the inner layer temperature in the two-zone model (which is an average temperature across the inner volume of the droplet) is lower than the temperature measured experimentally in the center. A part of the explanation is that, actually, the temperature profile found from the experiments is non-monotonic. Some regions in the droplet have a

temperature which is slightly lower than the center temperature. This behavior cannot be captured by the models at hand.

Comparing tests 1-4 and 5-8 shows that the simulations with the initial conditions computed based on the experimental data (i.e. tests 5-8) lead to a lower maximum peak value for the relative difference in the evaporative cooling (not shown due to space limitation). Moreover, this peak occurs faster. This results from the fact that, in this case, the different temperatures reach the saturation temperature faster. As a consequence, the difference between the isothermal and the two-zone model is smaller. When the temperature gradient is considered, the relative difference starts at a value different from zero as, even at $t = 0$ s, the surface and the average temperatures are not identical anymore.

Furthermore, the two sets of ‘numerical experiments’ i.e., tests 5-8 and 9-12, are compared. Considering the initial temperature gradient inside the droplet causes higher differences between the two models (not shown). Still the deviations depend on the way the initial conditions are computed from the experimental data.

The influence of the Biot number on the results is investigated in section 4.7. Nevertheless, the value of the critical Biot number has also been changed at this stage in order to aim for better agreement with the experimental data. From Fig. 5 it can be seen that a value of $Bi_{crit} = 0.28$ leads to a slower increase of the surface temperature, closer to the experimental data. Moreover, the temperature of the inner layer agrees better with the experimental center temperature. Still, it is worth noting that actually the inner temperature should be higher than the center temperature, as the inner temperature stands for the inner zone and thus also includes a part of the droplet that is at a higher temperature. One has to keep in mind that in the experiments heat is transported by conduction from the holder to the droplet, which has an impact on the temperature distribution and the droplet lifetime, as shown in [13, 14, 23]. This effect is not included in the in-house code. Therefore the simulation results and the experimental data should be compared with caution.

For the remainder of the simulations, it was decided to start with a uniform temperature of 20°C and a critical Biot number of 0.10 in order to study one single parameter at a time.

4.3 Influence of the ambient gas temperature

Figure 6 shows the impact of the ambient gas temperature on the relative difference between the two models for the heat exchange due to evaporation. The horizontal axis is made dimensionless using the droplet lifetime (which is almost the same whether the isothermal or the two-zone model is used). The same behavior is obtained for the different ambient temperatures, i.e., first, a higher cooling effect of the surrounding gas due to evaporation in the two-zone model and then, a lower value of the evaporative cooling rate compared to the isothermal model. Figure 6 shows clearly that the effect of the two-zone model increases (i.e., increased deviation) with an increasing ambient gas temperature.

Fig. 6. Influence of the ambient gas temperature on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $u_g = 3 \text{ m/s}$, $d_{a,0} = 3.06 \text{ mm}$, $T_{init} = 20 \text{ °C}$, $Bi_{crit} = 0.10$

4.4 Influence of the velocity

When the seen velocity, i.e., the relative velocity between the droplet and the surrounding air, increases, the Reynolds number increases correspondingly. This implies that the Sherwood and the Nusselt numbers will also rise. The impact of the Sherwood number is the same for the two approaches: it will promote the evaporation rate (see Eq. (1)) which results in a reduced droplet lifetime. The increase of the Nusselt number leads to a higher value of the convective coefficient and enhances convective heat transfer. This effect occurs similarly for the two approaches. However, the convective coefficient is used to determine the depth of the outer layer for the two-zone model. This implies that the increase of the velocity has an additional influence on the two-zone model as it reduces the depth of the evaporating layer. As the depth of this layer is smaller, the volume of liquid being heated is smaller and thus, the temperature of the layer rises faster. As a consequence, the influence of the two-zone model (in comparison to the isothermal model) increases as the velocity increases (see Fig. 7). Actually, the difference between the two surface temperatures and the two average temperatures (computed in the two models) is enhanced.

Fig. 7. Influence of the gas velocity on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $T_g = 500 \text{ °C}$, $d_{a,0} = 3.06 \text{ mm}$, $T_{init} = 20 \text{ °C}$, $Bi_{crit} = 0.10$

4.6 Influence of the initial diameter

Another simulation is run, where the initial diameter is decreased to 2 mm. The diameter is used in the definition of the Reynolds number of the droplet and its variation has the opposite effect to the change of the velocity described previously. Moreover, the diameter of the droplet is involved twice in the calculation of the convection coefficient (once directly and once indirectly

through the Nusselt number). It implies that the impact of the diameter is not straightforward. Nevertheless, from Fig. 8 it can be observed that a reduction of the initial diameter decreases the absolute value of the peaks. As expected, the effect of the two-zone model is reduced.

Fig. 8. Influence of the initial diameter on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$

4.7 Sensitivity analysis on the critical Biot number

The critical Biot number is directly proportional to the depth of the outer layer. Therefore, a sensitivity analysis on this parameter is carried out in order to study its effect on the overall behavior of the two-zone model. The lower the critical Biot number, the smaller the depth of the outer layer, and so is the volume of liquid in the evaporating layer. This implies that the surface temperature will increase faster with decreasing critical Biot number. Besides, the average temperature in the two-zone model is lower than in the isothermal model. This means that the influence of the two-zone approach is more pronounced with decreasing critical Biot number, as shown in Fig. 9. For the moment, it is difficult to speculate on the ‘most suitable’ value for the critical Biot number to be used in the two-zone model. A more detailed and comprehensive experimental dataset is required to do so with, preferably, less intrusive techniques that do not influence the thermal field inside the droplet.

Fig. 9. Influence of the critical Biot number on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$

4.8 Influence of the temperature dependence of the heat of vaporization

In the simulations above, the heat of vaporization of water was taken as constant at the boiling temperature ($L_v = 2256\text{ kJ/kg}$ at $100\text{ }^{\circ}\text{C}$). However, this quantity depends on the temperature,

which affects the rate of evaporation. A function, based on the data provided on [24], providing the heat of vaporization as a function of the surface temperature, has been implemented in the in-house code. Figure 10 (a) shows the time evolution of the heat of vaporization. From this figure it can be seen that this parameter decreases faster for the two zone model than for the isothermal model as the outer layer temperature increases faster than the isothermal temperature. Then the heat of vaporization tends to a constant value as the temperature reaches saturation temperature. The results show that, at some point, the temperature dependence of this parameter increases the relative difference of the evaporative cooling between the isothermal and the two-zone models by 6%. Therefore, inclusion of the temperature dependence of the latent heat of vaporization renders the evaporative cooling rate even more sensitive to the choice of the model (i.e., isothermal versus two-zone model).

Fig. 10. Zoom on the first 20% of the droplet lifetime of (a) the time evolution of the heat of vaporization and (b) the influence of the temperature dependence of the heat of vaporization on the relative difference between the two models for the evaporative cooling for $T_g = 500 \text{ }^\circ\text{C}$, $u_g = 3 \text{ m/s}$, $d_d = 3.06 \text{ mm}$, $T_{init} = 20 \text{ }^\circ\text{C}$, $Bi_{crit} = 0.10$

5. Conclusions

In this paper, a novel two-zone model for an evaporating droplet was presented. The simulation results of this model were compared to the simulation results obtained with the widely used isothermal model. The results were first compared to the experimental data obtained by Volkov and Strizhak [13] and [14]. It was found that the two-zone model did not improve the droplet lifetime, t_d , predictions displayed in [15], compared to the isothermal model. In fact, the differences in the predictions of t_d between the two models are marginal (less than 1%). The same comment could be made for the prediction of the saturation temperatures, which remained higher than the experimental values. Nevertheless, the analysis of the results obtained with the two different approaches showed that the choice of the model strongly affects the evaporative cooling rate by the droplet on the surrounding gas, particularly during the first seconds, which is the most important period in the lifetime of water droplets in the context of interaction with smoke and/or flames. The reason is that the implementation of the novel model allows to make a distinction between the surface temperature and the average droplet temperature. At the beginning of the simulations, the cooling effect of the surrounding gas due to the evaporation of the droplet is higher in the two-zone model compared to the isothermal approach.

A parametric study was completed in order to quantify the impact of some important parameters on the results obtained in the novel model. The differences between the two models are promoted

by an increase of the ambient gas temperature and/or an increase in the relative velocity. Furthermore, the effect of the two-zone model is more marked for larger droplets and when the temperature dependence of the heat of vaporization is considered. The results depend on the choice of the critical Biot number value. Therefore, more research on this value is required in order to further consolidate the present work. Finally, it is worth mentioning that this paper is a first analysis on this novel two-zone approach. The novel model is believed to offer a possibility to make a distinction between the average, the inner and the outer layer temperatures, which has an impact on the heat transfer between the droplet and the surroundings. However, more numerical and experimental work needs to be done before providing compelling evidence on the usefulness of the proposed two-zone approach.

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7. References

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Figure captions

Fig. 1. A schematic representation of a droplet using a two-zone approach

Fig. 2. A zoom on the initial time evolution of (a) the surface temperature, (b) the inner temperature, (c) the diameter, and (d) the evaporation rate¹ for test 3, i.e. $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$

Fig. 3. Time evolution of the evaporative cooling of the droplet on the surrounding gas and the relative difference between the two models for test 3: $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$

Fig. 4. Comparison of the initial temperature profile for the experimental data, the isothermal model and the two-zone model for test 7, i.e. $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $Bi_{crit} = 0.10$

Fig. 5. Comparison of the time evolution (the first 5s) of the temperature for the isothermal model (yellow), for the two-zone model without an initial temperature gradient (purple), for the two-zone with an initial temperature gradient (green), for the two-zone model with an initial temperature gradient and a value of 0.28 for the critical Biot number (grey), and the experimental data (black) for the conditions $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$

Fig. 6. Influence of the ambient gas temperature on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$

Fig. 7. Influence of the gas velocity on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $T_g = 500\text{ }^{\circ}\text{C}$, $d_{d,0} = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$

Fig. 8. Influence of the initial diameter on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$

Fig. 9. Influence of the critical Biot number on the relative difference between the two models for the evaporative cooling over (a) the entire droplet lifetime and (b) zoom on the first 20% of the lifetime for $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_{d,0} = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$

Fig. 10. Zoom on the first 20% of the droplet lifetime of (a) the time evolution of the heat of vaporization and (b) the influence of the temperature dependence of the heat of vaporization on the relative difference between the two models for the evaporative cooling for $T_g = 500\text{ }^{\circ}\text{C}$, $u_g = 3\text{ m/s}$, $d_d = 3.06\text{ mm}$, $T_{init} = 20\text{ }^{\circ}\text{C}$, $Bi_{crit} = 0.10$