

Research Paper

A 3rd-order polynomial temperature profile model for the heating and evaporation of moving droplets

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HIGHLIGHTS

- A new liquid model for heating and evaporation of moving droplets is proposed.
- 3rd-order polynomial profile is assumed for internal temperature of droplet.
- Internal circulation of droplet is approximated by Hill's spherical vortex.
- Droplet internal temperature distribution is correctly reflected by new model.
- New model is more efficient than thermal conductivity models (CL and ETC models).

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ABSTRACT

Droplet heating and evaporation is of fundamental importance in various engineering applications. Based on the assumption that droplets' internal temperature follows a third-order polynomial distribution, a new liquid phase model is proposed, taking into account both temperature gradient and internal circulation inside the droplet in terms of Hill's spherical vortex. The new liquid model and other commonly used liquid models are compared with the experimental data outlined in the literature. The internal temperature predicted by the new model matches the experimental data of an *n*-Decane droplet heating best, whereby the enhancement of heat transport by internal circulation is correctly reflected. In comparison, other models always predict the monotonic variation of internal temperature during the initial heating period, which deviates widely from the experimental data. The new model displays the best performance with regard to predicting droplet evaporation in the later vaporizing period, whereas the parabolic temperature profile model and conduction limit model significantly underestimate and overestimate the droplet evaporation rate, respectively. The CPU requirement for the new model is far less than that for the conduction limit model and the effective thermal conductivity model with an order of magnitude, which shows its potential for implementation into CFD codes.

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1. Introduction

As a common physical phenomenon, droplet heating and vaporization are of fundamental importance in various engineering applications [1–3]; for example, the combustion efficiency of the internal combustion engine is strongly affected by the droplet vaporization rate and mixing ability with the ambient gas flow [4–6]; the therapeutic outcome and cooling efficiency of cryogen spray cooling are influenced strongly by the vaporization of droplets in laser dermatology [7–10]; the efficiency of heat exchange

is dominated by droplet vaporization in a cooling tower [11,12], etc.

The importance of developing a single droplet model with sufficient accuracy and high computational efficiency in describing droplet heating and evaporation has been well recognized [4,13,14]. However, there is a tradeoff between accuracy and computational efficiency. As classified by Sazhin et al. [15], the well-known liquid phase models for droplet heating and evaporation in order of ascending complexity are as follows: (1) the lumped liquid model based on the assumption of uniform temperature distribution within the whole droplet; (2) the model taking into account heat transfer by finite thermal conductivity but no recirculation inside the droplet (conduction limit model); (3) the model considering heat transfer by both conduction and recirculation inside the

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Nomenclature

B_M	spalding mass transfer number
B_T	spalding heat transfer number
c_p	specific heat capacity (J/(kg·K))
h	convective heat transfer coefficient (W/(m ² ·K))
L	latent heat of evaporation (J/kg)
$\dot{m}$	total droplet vaporization rate (kg/s)
Nu	Nusselt number
Pe	Peclet number
Pr	Prandtl number
q	heat flux (W/m ²)
Re	Reynolds number
r	droplet radius (m)
$\dot{r}_s$	decreasing rate of droplet radius (m/s)
Sc	Schmidt number
Sh	Sherwood number
t	time (s)
T	temperature (K)
u	velocity (m/s)
U_s	maximum velocity on the droplet surface (m/s)
V_r	radial component of liquid velocity (m/s)
V_θ	angular component of liquid velocity (m/s)
Y	mass fraction

Greek symbols

λ	thermal conductivity (W/(m·K))
Γ	binary diffusion coefficient (m ² /s)
φ	non-dimensional stream function
ρ	density (kg/m ³)
μ	dynamic viscosity (N·s/m ²)
χ	coefficient of conductivity correction
η	dimensionless coordinate

Subscripts

c	convection
eff	effective
g	gas property on the droplet surface
gl	ratio of parameters of gas to liquid
l	liquid
p	constant pressure
s	droplet surface
v	vapor
0	initial state
∞	far from the droplet surface
—	average

droplet with an amplified liquid thermal conductivity (effective thermal conductivity model); (4) the vortex model taking into account the recirculation in terms of vortex dynamics; and (5) the model based on the full solution of the Navier-Stokes equation. The lumped model is widely used in most CFD codes owing to its high computational efficiency, since it is unnecessary to calculate the internal temperature gradient within the droplet (0-dimension model). Nevertheless, the disadvantage of this model is obvious: if the liquid thermal conductivity is insufficient, then it is important to take into account the transient heating of the droplet in cases of large droplets and long droplet lifetime. As demonstrated by Sazhin et al. [15,16], transient heating and the temperature gradient inside droplets are quite important for the calculation of fuel spray in engines if liquid break-up is involved, which results in a large decrease in the droplet evaporation time. Under these conditions, it might be possible to employ the liquid conductivity models (conduction limit and effective thermal conductivity models) to calculate the complicated differential equations of heat conduction within droplets, ignoring recirculation. However, the computational efficiency is far less than the lumped model would provide. The vortex and full Navier-Stokes models are extremely complex and inappropriate for the implementation of CFD codes in the near future due to their huge CPU requirement, and the need for a deeper understanding of physics during droplet heating and vaporization, as in the basic models.

Usually, it is unnecessary to define the specific temperature distribution within droplets in the CFD calculation for sprays. Alternatively, heat and mass transfer is closely related to both droplet surface temperature and average temperature. Dombrovsky and Sazhin [17] developed a parabolic temperature profile model, in which the internal temperature was approximated to a parabolic form. This model was less accurate than either the conduction limit or effective thermal conductivity model, but offered comparable computational efficiency to the lumped model. Further, Sazhin et al. [18] proposed a semi-empirical analytical solution concerning droplets' internal temperature distribution based on the conduction limit and effective thermal conductivity models. This

model is more accurate than the parabolic temperature profile model, although its analytical solution is quite complicated, with less computational efficiency. Generally, the liquid models derived from single heat conduction within droplets are usually suitable for conditions with very a low Reynolds number (smaller than 1) [19].

In fact, if relative motion exists between the droplet and surrounding gas, the viscous shear stress acting on the droplet surface will lead to internal circulation inside the droplet. As a result, the rate of droplet heating and evaporation as well as the motion and species transfer will be enhanced. The droplet surface and center will be heated before the middle region during the transient heating period due to the internal circulation [18]. The importance of internal circulation, especially for multicomponent droplet evaporation, has been recognized previously [20–22]. However, none of the available models has taken this kind of transient heating into account.

This paper aims to develop a new liquid phase model for droplet heating and evaporation, based on a more reasonable temperature distribution inside the droplet. The temperature gradient and internal circulation inside the droplet are incorporated through the introduction of Hill's spherical vortex. The predictions and the findings of the experimental data regarding the performance of the new model and other commonly used liquid models are compared, for both heating and evaporation. The computational efficiency for these models is also examined.

2. Droplet model for heating and vaporization

2.1. Physical consideration

To reduce the complexity and eliminate the effect of drag force on droplet heating and evaporation, we consider a suspended liquid droplet with a pure component that is subjected to a convective gas flow, which is consistent with the experimental conditions described in Section 4. Several assumptions are made, as follows:

- (1) The droplet is spherically symmetrical and one dimensional.
- (2) The liquid/gas interface is at local equilibrium, with vapor saturated at the droplet surface temperature.
- (3) The ambient gases are not soluble in droplets due to the small liquid binary mass diffusivity.
- (4) The Soret and Dufour effects are ignorable.
- (5) Radiation is neglected.

2.2. Heat and mass transfer on the droplet surface

According to Fick's laws of mass diffusion and Stefan's flow effect, the droplet vaporization rate for the total droplet surface can be written as:

$$\dot{m} = -2\pi r_s \bar{\rho}_g \Gamma Sh B_M \quad (1)$$

where Γ , Sh , $\bar{\rho}_g$ and r_s are the binary diffusion coefficient of the liquid vapor in the ambient gas, the Sherwood number, the average density of the mixture of gas near the droplet surface, and the droplet radius, respectively. B_M is the Spalding mass transfer number, which is calculated as $B_M = Y_{v,s}/(1 - Y_{v,s})$. $Y_{v,s}$ is the vapor mass fraction on the droplet surface and can be obtained from the Clausius-Clapeyron equation [23]. The driving force of the mass transfer B_M in Eq. (1) is less common than $\ln(1 + B_M)$ which tends to be adopted in the previous literature. It is found that B_M is more suitable for the transient heating and evaporation without the limitation of the quasi-steady assumption in its derivation [23].

The convection heat flux q_c between the droplet surface and the ambient gas is given by:

$$q_c = h(T_g - T_s) = \frac{\bar{\lambda}_g Nu}{2r_s} (T_g - T_s) \quad (2)$$

where h , Nu and $\bar{\lambda}_g$ are the heat transfer coefficient, the Nusselt number and the average thermal conductivity of the gas mixture near the droplet surface, respectively. T_g and T_s are the temperature of the ambient gas and droplet surface, respectively.

From mass equation (1) and energy equation (2), it appears that the mass and heat transfer between the droplet surface and the ambient gas are significantly sensitive to the selection of the Nu and Sh number. In fact, a multitude of correlations of the Nu and Sh number for droplet evaporation exists, derived from the analytical analysis, numerical simulation and experiment measurements [24–30]. The selection of a suitable one is an essential step for the calculations employed in many industrial applications. The difference between the various correlations of the Nu and Sh number has been reviewed by researchers under different conditions [15,23,30]. It has been demonstrated that these correlations predicted virtually identical results for droplet evaporation in cases of low evaporation rate, while significant deviations were found among the predictive results at the large evaporation rate. Recently, we proposed a new correlation of the Nu and Sh number, incorporating a blowing effect and a convective effect. It predicted droplet evaporation well at the various evaporation rates [30]. Thus, this correlation was adopted to calculate the heat and mass transfer on the droplet surface, which is given as follows,

$$Nu = (1 + B_T)^{-\frac{2}{3}} \left(2 + 0.552 Re_d^{1/2} Pr_g^{1/3} \right) \quad (3)$$

$$Sh = (1 + B_M)^{-\frac{2}{3}} \left(2 + 0.552 Re_d^{1/2} Sc_g^{1/3} \right) \quad (4)$$

where Re_d , Pr_g and Sc_g are the Reynold number of the droplet and the Prandtl and Schmidt number for gas, respectively. Re_d , Pr_g and Sc_g are calculated as $Re_d = 2r_s \bar{\rho}_g u_g / \bar{\mu}_g$, $Sc_g = \bar{\mu}_g / \bar{\rho}_g \Gamma$ and $Pr_g = \bar{\mu}_g \bar{c}_{pg} / \bar{\lambda}_g$, where u_g , $\bar{\mu}_g$ and $\bar{c}_{pg}$ are the ambient gas velocity, average dynamic viscosity and specific heat capacity of the gas mixture. B_T is the Spalding heat transfer number, which is calculated as

$B_T = c_{pl}(T_g - T_s)/L_v$, where c_{pl} and L_v are the specific heat capacity for the liquid and the latent heat for evaporation, respectively.

The average thermophysical properties of the gas mixture ($\bar{\rho}_g$, $\bar{\lambda}_g$, $\bar{\mu}_g$ and $\bar{c}_{pg}$) near the droplet surface are estimated by the reference temperature and vapor concentration. Yuan and Chen recommended the “1/3” rule for the reference value, which is widely adopted in previous studies [31]. Hence, it is employed to calculate the average thermophysical properties of the gas mixture.

2.3. The liquid phase model

In this section, the commonly used liquid models are described briefly, i.e. the lumped, the conduction limit model, the effective thermal conductivity and the parabolic temperature profile model. Then, the new model will be described in detail.

(1) Lumped model

For the lumped model, the droplet temperature is assumed to be uniform throughout the whole droplet. Therefore, the energy equation for droplet heating is given as follows:

$$\frac{dT}{dt} = \frac{3L\dot{r}_s}{c_{pl}r_s} + \frac{3h(T_g - T_s)}{\rho_l c_{pl}r_s} \quad (5)$$

where ρ_l is the liquid density, $\dot{r}_s$ is the decreasing rate of the droplet radius, and $\dot{r}_s = -\Gamma \bar{\rho}_g Sh B_M / 2r_s$.

(2) Conduction limit model (CL model) and effective thermal conductivity model (ETC model)

The conduction limit model takes the temperature gradient within the droplet into account. It assumes that there is no internal circulation in the droplet. Therefore, the transient heat conduction equation in the droplet can be solved as follows,

$$\frac{\partial T}{\partial t} = \frac{1}{\rho_l c_{pl}} \frac{\lambda_l}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial T}{\partial r} \right) \quad (6)$$

where λ_l is the thermal conductivity of the liquid. The boundary and initial conditions are:

$$\frac{\partial T}{\partial r} \Big|_{r=r_s} = \frac{1}{\lambda_l} [\rho_l L \dot{r}_s + h(T_g - T_s)] \quad (7)$$

$$\frac{\partial T}{\partial r} \Big|_{r=0} = 0 \quad (8)$$

$$T(t=0, r) = T_0 \quad (9)$$

where T_0 is the droplet's initial temperature.

In the effective thermal conductivity model, the effect of internal circulation on droplet heating has been taken into account. However, the real circulation equation in the droplet will not be solved in this model. Alternatively, the liquid thermal conductivity λ_l is replaced by the amplified effective thermal conductivity $\lambda_{\text{eff}} = \chi \lambda_l$. The coefficient of χ can be approximated by $\chi = 1.86 + 0.86 \tanh[2.225 \log_{10}(Pe_l/30)]$, which varies from 1 to 2.72 [24].

(3) Parabolic temperature profile model (2nd-order model)

This model is based on the assumption of the parabolic temperature profile inside the droplet. The key parameters are the surface temperature T_s and the average temperature $\bar{T}$. Firstly, $\bar{T}$ is defined as follows,

$$\bar{T} = \frac{3}{r_s^3} \int_0^{r_s} r^2 T(r) dr \quad (10)$$

Then the new energy equation of droplet heating can be derived through combining Eqs. (5)–(7),

$$\frac{d\bar{T}}{dt} = \frac{3r_s}{r_s} \left(T_s - \bar{T} + \frac{L}{c_{pl}} \right) + \frac{3h}{\rho_l c_{pl} r_s} (T_g - T_s) \quad (11)$$

If the temperature throughout the droplet is uniform, i.e. $T = T_s = \bar{T}$, Eq. (11) will be reduced to Eq. (5), i.e., the lumped model.

For the parabolic temperature profile model, the temperature distribution inside the droplet is assumed to take the form: $T(r) = a + br + cr^2$. The coefficient b should be equal to zero, since it must satisfy Eq. (8). Therefore, the internal temperature distribution can be simplified as: $T(r) = a + cr^2$. This indicates that the internal temperature must comply with the monotonic variation in the radius range from 0 to r_s , since the temperature is symmetric about the droplet center ($r = 0$). Incorporating Eqs. (7) and (10), T_s can be derived as follows,

$$T_s = \frac{\bar{T} + 0.1\lambda_{gl}NuT_g}{1 + 0.1\lambda_{gl}Nu} + \frac{2\rho_l L r_s}{\lambda_l(1 + 0.1\lambda_{gl}Nu)} \quad (12)$$

where λ_{gl} is the ratio of gas thermal conductivity to liquid conductivity, $\lambda_{gl} = \lambda_g/\lambda_l$. Eqs. (11) and (12) provide the full solution of droplet heating during evaporation. In comparison with the lumped model, the final step is to solve the surface temperature at each iteration.

(4) New liquid phase model (3rd-order model)

As a droplet is exposed to a gas flow, the shear stress acting on the droplet surface will result in internal circulation inside the droplet, which can be approximately described by Hill's spherical vortex (shown in Fig. 1) [24,32,33]. This internal circulation will enhance the heat transport from the droplet surface to the center, leading to a relatively low temperature at the center of the vortex. Naturally, the aforementioned parabolic temperature profile is unsuitable for predicting the temperature distribution at this condition.

Alternatively, this paper proposed a 3rd-order polynomial temperature profile to describe the internal temperature distribution, which matches this kind of temperature variation caused by the internal circulation. As shown in Fig. 2, the high temperature at the droplet center and low temperature at the vortex center induced by internal circulation can be reasonably represented by

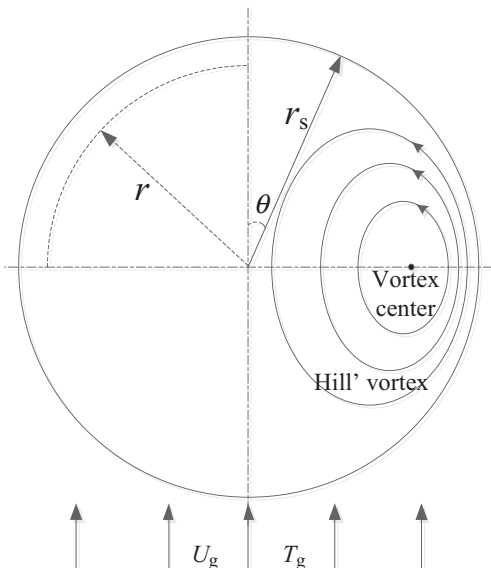


Fig. 1. Schematic of Hill's spherical vortex inside the droplet [34].

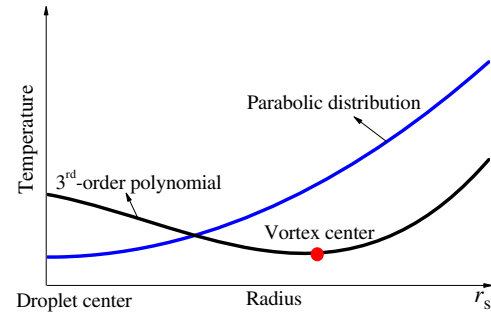


Fig. 2. Schematic of different temperature distributions inside the droplet.

the 3rd-order polynomial profile, whereas the parabolic profile only gives the monotonic temperature variation with the lowest temperature in the droplet center. Therefore, the 3rd-order polynomial profile is adopted to replace the parabolic one in this new model. It is given by: $T(r) = a + br + cr^2 + dr^3$. Similarly, the new temperature profile equation should satisfy Eqs. (7)–(10). However, the new model has four completely unknown coefficients, i.e. a , b , c and d . Based on Hill's vortex, another condition is employed to solve this temperature profile. The instantaneous velocities inside the droplet can be calculated by the Hill's spherical vortex solution,

$$V_\theta = U_s \left(1 - \frac{2r^2}{r_s^2} \right) \sin \theta \quad (13)$$

$$V_r = U_s \left(1 - \frac{r^2}{r_s^2} \right) \cos \theta \quad (14)$$

where V_r , V_θ and U_s are the radial and angular components of the liquid velocity inside the droplet, and the maximum velocity on the droplet surface. It is noted that there exists a stagnation point in the vortex center, where V_r and V_θ are all equal to zero. Additionally, the non-dimensional stream function (φ) at the vortex center is also zero [34],

$$\varphi = 1 - 4 \left(\frac{r}{r_s} \right)^2 \left[1 - \left(\frac{r}{r_s} \right)^2 \right] \sin^2 \theta = 0 \quad (15)$$

Hence, the position of the vortex center can be determined through Eqs. (13)–(15): $r = 0.707r_s$ and $\theta = 90^\circ$ or 270° . The heat transfer inside the droplet will be greatly enhanced by the internal circulation. However, it is found that the temperature of the vortex center is minimal, due to stagnation [13],

$$\left. \frac{\partial T}{\partial r} \right|_{r=0.707r_s} = 0 \quad (16)$$

By incorporating Eqs. (7), (8), (10) and (16), T_s for the 3rd-order temperature profile model can be derived as:

$$T_s = \frac{\bar{T} + 0.043\lambda_{gl}NuT_g}{1 + 0.043\lambda_{gl}Nu} + 0.086 \frac{\rho_l L r_s}{\lambda_l(1 + 0.043\lambda_{gl}Nu)} \quad (17)$$

Eqs. (11) and (17) provide the full solution of droplet heating during its evaporation period for the new liquid phase model. Since the 3rd-order polynomial temperature profile can reflect the influence of the internal circulation in terms of Hill's spherical vortex on droplet heating, it is expected to outperform the 2nd-order parabolic temperature profile model.

3. Numerical method

For the lumped, parabolic temperature profile and new 3rd-order liquid phase models, it is unnecessary to solve the complex differential equation of heat conduction inside the droplet, since they are all “0-dimensional” problems. From energy Eqs. (5) and (11), it can be seen that the droplet temperature (T) or average temperature ($\bar{T}$) is only a function of time (t). A fully implicit iterative method is used to solve mass Eq. (1) and energy Eq. (5) or (11). The time step (Δt) will be updated to $(t + \Delta t)$ as the convergence is achieved at the conditions of $|T^j - T^{j+1}| < 10^{-7}$ K and $\frac{m^j - m^{j+1}}{m^j} < 10^{-7}$, where j is the iteration number.

For the conduction limit and effective thermal conductivity models, it is necessary to solve the heat conduction equation within the droplet. To account for the droplet surface regression due to evaporation, the spatial coordinate is transformed to fix the droplet surface [35,36], so the dimensional coordinate r is changed to the dimensionless coordinate η , where $\eta = r/r_s$, $0 \leq \eta \leq 1$. Thus, Eqs. (6)–(8) are transformed as follows,

$$\frac{\partial T}{\partial t} = \frac{\lambda_l}{\rho_l c_{pl} r_s^2 \eta^2} \frac{\partial}{\partial \eta} \left(\eta^2 \frac{\partial T}{\partial \eta} \right) + \eta \frac{\dot{r}_s}{r_s} \frac{\partial T}{\partial \eta} \quad (18)$$

$$\frac{\partial T}{\partial \eta} \Big|_{\eta=1} = \frac{r_s}{\lambda_l} [\rho_l L r_s + h(T_g - T_s)] \quad (19)$$

$$\frac{\partial T}{\partial \eta} \Big|_{\eta=0} = 0 \quad (20)$$

The fully implicit scheme backwards in time and a control volume integral method are used to discretize the above governing equations, before being solved with a TDMA algorithm [37]. The time step Δt and grid size $\Delta \eta$ are 10^{-5} s and 0.001, which are adequately small for the results' independence.

4. Results and discussions

All of the models are validated by the previous experimental data about droplet heating and evaporation by Wong and Lin [19]. In their experiment, an *n*-Decane droplet was hung in a very hot gas flow with a temperature of 1000 K and atmospheric pressure. The droplet's initial diameter and temperature were about 2 mm and 315 K respectively, and the initial Reynolds number was 17. The variations in the droplet's diameter and temperature versus time were recorded using a video recorder and thermocouple. In this paper, the initial conditions for all model simulations were identical to those in the above experimental conditions. The predicted results of droplet vaporization and heating by all liquid phase models will be compared with the experimental data. Some thermophysical properties of *n*-Decane were presented in Ref. [24]. The others are calculated by NIST-REFPROP7.1.

In the following sections, the parabolic temperature profile model and the new model are abbreviated as the 2nd-order model and 3rd-order model. The conduction limit and effective thermal conductivity models are abbreviated as the CL model and the ETC model, respectively.

4.1. Droplet heating

Fig. 3 shows the droplet's temperature, as predicted by different liquid models and the experimental data [19] at two locations (a) $r/r_s = 0$ and (b) $r/r_s = 0.6$ within the droplet as a function of time. Fig. 3(a) shows that the prediction by the 3rd-order model matches the experimental data best at the droplet center, whereas all of the other models underestimate the droplet temperature, since the

internal circulation in the droplet greatly enhances the heating in the droplet center. The lumped model treats the whole droplet as being heated simultaneously. As a result, the temperature of the droplet center increases more rapidly than those predicted by the CL and ETC models, in which heat transfer towards the droplet center occurs only through heat conduction or the correction of the amplified heat conduction. However, the center temperature predicted by the 2nd-order model rises sharply at the beginning of the heating period, which is much lower than the initial temperature. For the other location ($r/r_s = 0.6$), different trends are observed. It seems that the temperature predicted by the lumped model matches the experimental data best, and the 3rd-order model slightly underestimates this temperature, probably due to its proximity to the vortex center (stagnation point) where the heating enhancement by circulation is at its weakest. The CL and ETC models still heavily underestimate the droplet temperature, whereas the 2nd-order model produces far better results than that at the center.

Fig. 4 shows a comparison between the experimental data and the simulation results for the internal temperature of the droplet with respect to the dimensionless radius r/r_s at different evaporation times (a) $t = 0.4$ s, (b) $t = 0.8$ s, (c) $t = 1.2$ s, and (d) $t = 2.4$ s. For the experimental data reported by Wang and Lin [19], the temperature does not present the monotonic variation along the droplet radius. Alternatively, the minimum temperatures for four different instants seem to occur around $r/r_s = 0.7$, which is relatively close to the vortex center ($r/r_s = 0.707$). The core temperature of the droplet is somewhat higher than the minimum temperature. However, these are slightly lower than the surface temperatures, especially for the initial heating period. This internal temperature distribution pattern apparently demonstrates the existence of internal circulation due to convective gas flow, which indeed enhances the heat transport from the droplet surface to the interior. For the simulation results when using different liquid models, these can probably be divided into two groups based on their performance. One may be called the monotonic model, including the 2nd-order model as well as the CL and ETC models. The predicted temperature by this group decreases monotonically towards the droplet center. Additionally, the results deviate greatly from the experimental data since only heat conduction is considered. They greatly underestimate the droplet's core temperature especially at the beginning of the heating period. The 2nd-order model almost predicts the lowest core temperature, whereas the opposite applies to the highest surface temperature. This wide deviation from the experimental data indicates that the 2nd-order model based on the parabolic temperature profile inside the droplet may not be applicable for predicting the internal temperature of the moving droplet.

The other group is the 3rd-order model, which can be seen as the simplified vortex model. The predicted internal temperature agrees quite strongly with the experimental data at the very beginning ($t = 0.4$ s) and the stage close to the stable heating ($t = 2.4$ s), which is attributed to the internal circulation concerned. As the time increases to $t = 0.8$ s and $t = 1.2$ s, the discrepancy between the prediction and the experimental data appears to increase, due to the assumption of the isothermal streamline in the Hill's vortex. However, this demonstrates that the temperature along the streamline was far from isothermal during the heating period [38,39]. Nevertheless, the 3rd-order model is far better at predicting the internal droplet temperature compared with the other models from the perspective of the whole transient heating period. Finally, it should be mentioned that one must exercise caution when the new model is adopted for highly viscous liquid such as slurry fuel and heavy oil, since this increased viscosity retards the internal circulation and consequently heat transport rate.

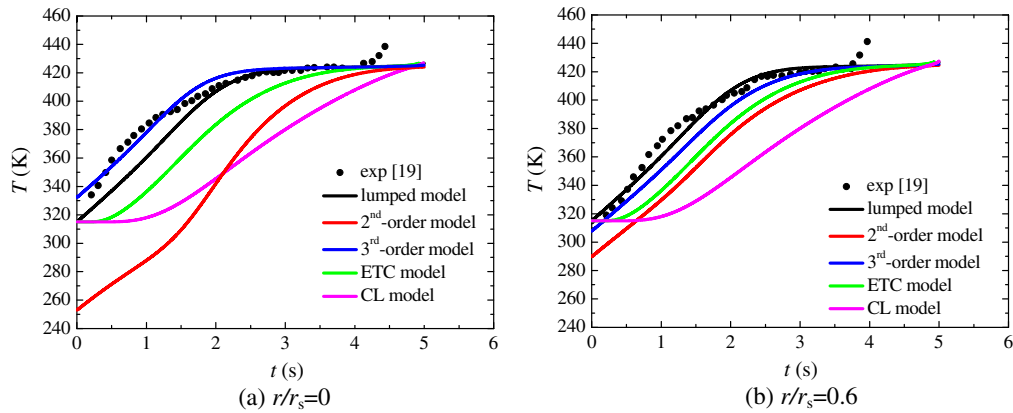


Fig. 3. Droplet temperature at two locations ($r/r_s = 0$ and $r/r_s = 0.6$) in the droplet as a function of time by model predictions and experimental data.

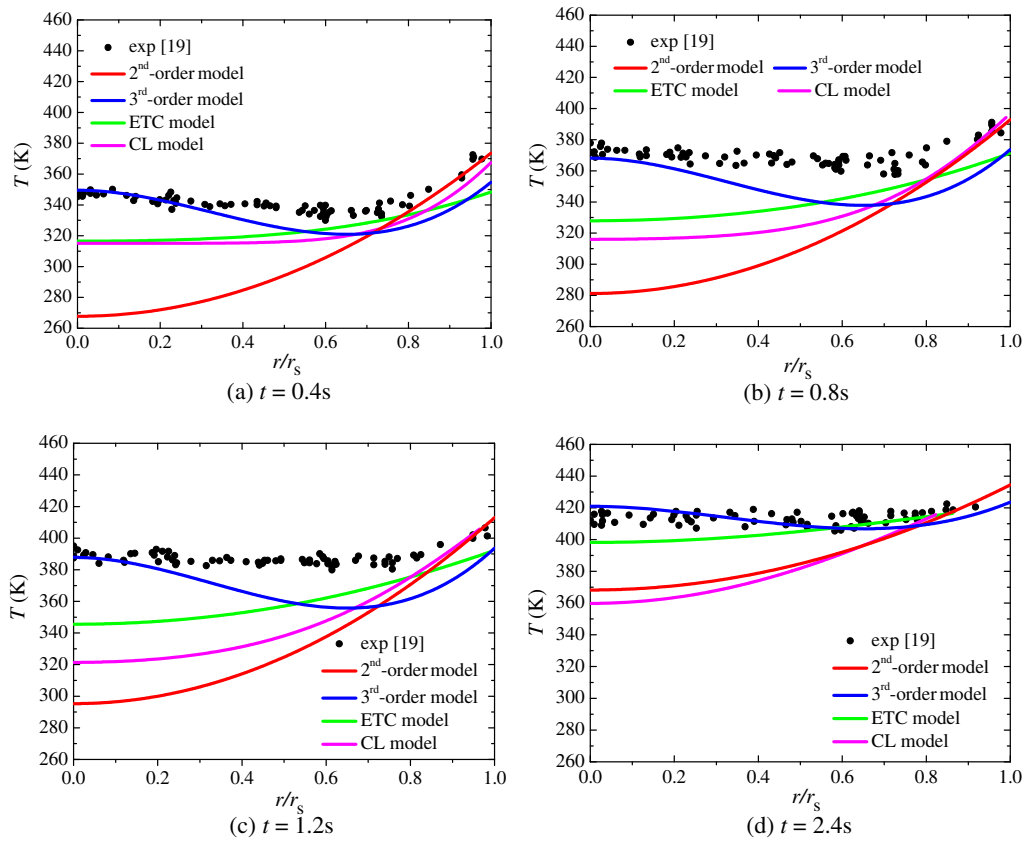


Fig. 4. Comparison between the experimental data and simulation results for the droplet internal temperature variations with respect to the dimensionless radius (r/r_s) at varied evaporation times (a) $t = 0.4$ s, (b) $t = 0.8$ s, (c) $t = 1.2$ s, and (d) $t = 2.4$ s.

Fig. 5 presents the surface temperature of the *n*-Decane droplet as a function of time for different models. Generally, the surface temperature calculated by all models increases rapidly in the first approximate 2 s before approaching a stable temperature of about 425 K, which is lower than the boiling point of about 447.7 K. However, the histories of reaching the stable temperature vary significantly for various models. The lumped model produces the smallest increasing rate of surface temperature, because the input heat from ambient hot gas is used to enhance the whole droplet simultaneously. Nevertheless, the input heat firstly heats the outer layer of the droplet, then the internal liquid will be heated gradually through heat conduction from the high temperature outer layer for the CL and ETC models. Consequently, the surface temper-

ature increases more rapidly than that of lumped model during the initial heating period. As we know, the heat conduction rate depends on the liquid thermal conductivity when the other conditions are the same. Therefore, the surface temperature predicted by the CL model has the largest increasing rate since the input heat is firstly accumulated on the outer layer due to the low conductivity. Correspondingly, its surface temperature is last to reach the stable temperature due to the low mixing rate. For the 2nd- and 3rd-order models, the former always predicts the highest surface temperature during the whole heating period. There exist certain temperature jumps at the beginning of the initial heating period, due to the assumption of the temperature distribution within the droplet. The temperature jumps can be calculated through Eqs. (12)

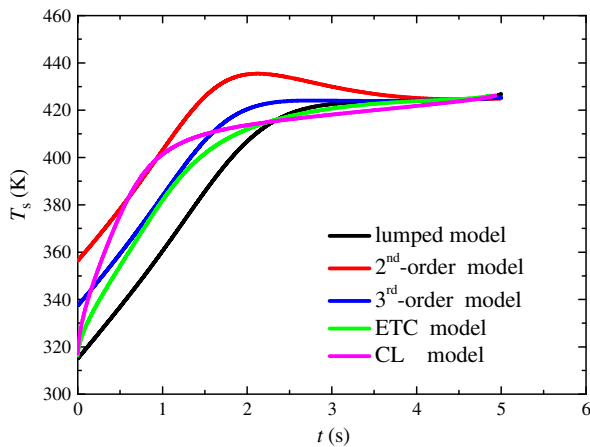


Fig. 5. Surface temperature T_s of n -Decane droplet versus time by different models.

and (17), where the 315 K initial average temperature causes about a 356 K and 337 K surface temperature for the 2nd- and 3rd-order models, respectively. What's more, a much higher surface temperature even emerges before it reaches the steady stage for the 2nd-order model. This is mainly caused by the quite large initial temperature jump. Finally, it is found that the stable temperature is unaffected by the liquid models.

The average temperatures of the droplet versus the time are illustrated in Fig. 6. The average temperature is a relatively important parameter since it reflects the state of the whole droplet's temperature. In contrast with the surface temperature, all of the predicted average temperatures follow similar trends, except for the LC model. They first increase quickly during the initial heating period, and then their increasing rates become slower until the stable temperature is reached. For the LC model, the magnitude of the average temperature increase is far smaller than the others during the whole evaporation period, owing to the lowest mixing rate. The average temperature reveals an approximately linear increase with time. Overall, the lumped model, the 2nd- model and the 3rd-order model can be regarded as the rapid mixing model as they do not solve the internal heat conduction equation within the droplet, which leads to sharper rises in the average temperature than occurs with the conduction models (including the LC and ETC models).

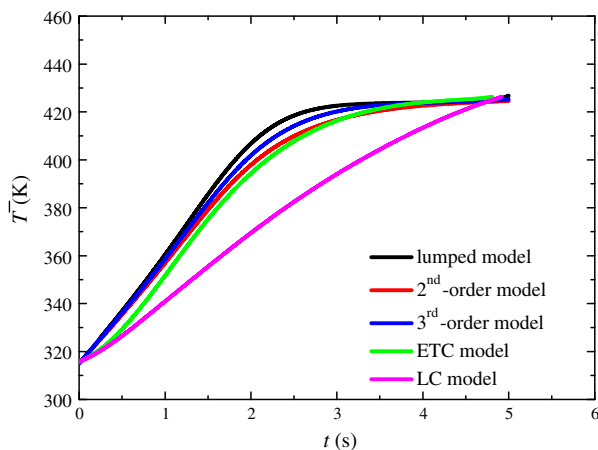


Fig. 6. Average temperature $\bar{T}$ of n -Decane droplet versus time for different models.

4.2. Droplet evaporation

A comparison between the experimental data and simulation results of the droplet diameter as a function of time is shown in Fig. 7. During the initial transient heating period of about the first 2 s, the " D^2 " law is invalid, and then it transfers to the linear " D^2 " reduction regime for the experimental data. Generally, all models predict a similar variation in the trend of droplet diameter from the perspective of the whole droplet vaporizing time. However, a large discrepancy exists. The 2nd-order model predicts the smallest droplet evaporation rate, whereas the CL model overestimates the droplet evaporation the most. The predictions by the other three models lie between those by the 2nd-order and the CL models, which are closer to the experimental data. Overall, the 3rd-order model shows the best performance in predicting droplet evaporation during the later steady vaporizing stage, whereas the result produced by the ETC model agrees most closely with the experimental data at the beginning of the initial heating period. As might be expected, the droplet evaporation rate depends significantly on the surface temperature. A higher surface temperature will lead to a greater droplet evaporation rate. This is indeed true for the CL and ETC models shown in Figs. 2 and 6. However, the opposite applies to the lumped, 2nd- and 3rd-order models, i.e., a higher surface temperature causes a lower evaporation rate, even though the surface temperature is used to evaluate the heat and mass transfer on the droplet surface in these models. The relationship between the evaporation rate and droplet average temperature was carefully examined. A higher average temperature leads to a greater evaporation rate, which means that the evaporation rate is determined by the droplet's average temperature for these three models. This may be explained by the fact that they have quite similar energy equations for droplet heating, although the temperature gradient and circulation in the droplet are taken into account.

In order to show the relationship between droplet evaporation rate and its temperature clearly, the surface temperature for the CL and ETC models and the average temperature for the lumped model, the 2nd- and 3rd-order models are rearranged and plotted in Fig. 8. It is found that the evaporation rate shown in Fig. 7 perfectly corresponds to the temperature presented in Fig. 8.

From the predictive results of droplet heating and evaporation by different liquid models, it was found that droplet stable temperature were the same and were not depended on the liquid model, however different liquid models predicted much different temperature increase rates at the transient heating period shown in

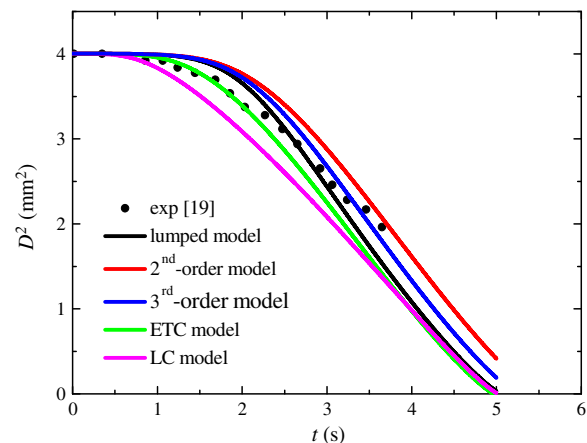


Fig. 7. Comparison between the experimental data and the simulation results of the droplet's diameter variation as a function of time.

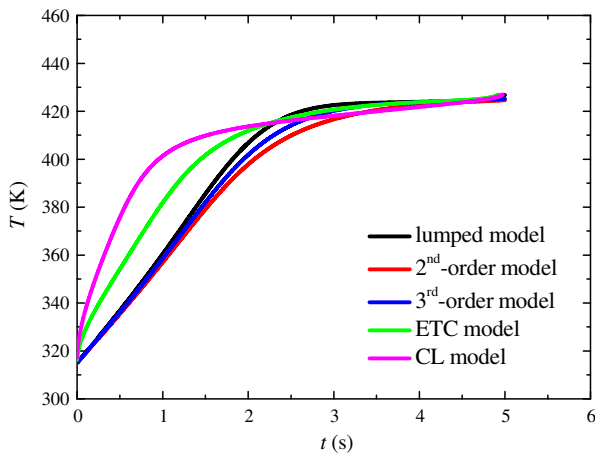


Fig. 8. Average temperature of the lumped model, 2nd- and 3rd-order models, and the surface temperature of the CL and ETC models for the *n*-Decane droplet versus time.

Figs. 4–6. On the other hand, it was noticed that droplet evaporation rate was governed by droplet transient surface temperature for CL and ETC models and by average temperature for lumped, 2nd-order and 3rd-order models shown in Figs. 7 and 8. Therefore, the liquid model also has very important effect on droplet heating and evaporation compared to that of the gas phase model about *Nu* and *Sh* numbers. Much care should be taken as they are applied in the industrial applications.

4.3. Computational efficiency

Fig. 9 presents the CPU time for the different models required for computing 5 s' evaporation on a laptop (Intel(R) Core(TM) CPU@2.5 GHz). As shown in the Figure, the lumped model is the most efficient, requiring the least time for the computation. The CPU requirements for the ETC and CL models are more than an order of magnitude larger than those for the 2nd- and 3rd-order models. This allows us to recommend the 3rd-order model for practical applications, including its possible implementation in CFD codes. Although the 3rd-order model has lower computational efficiency than the lumped model, this is acceptable due to its contribution towards improving the predicted droplet's internal temperature.

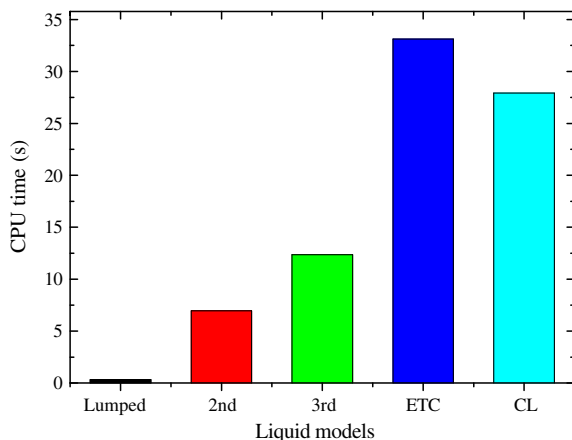


Fig. 9. CPU time for different models required for the computation of 5 s' evaporation.

5. Conclusions

A new liquid phase model is proposed based on the assumptions of the 3rd-order polynomial temperature distribution and Hill's vortex model inside the droplet, in which the temperature gradient and internal circulation are taken into account. The new model is validated by the previous experimental data for both droplet heating and evaporation, and compared with other common models. The main conclusions can be summarized as follows,

- (1) The temperature gradient actually exists and internal circulation indeed enhances the heat transport from the droplet's surface to the interior during the droplet's initial heating period. The new 3rd-order model provides a far better prediction of the internal temperature distribution than the other models. The heat transportation from the droplet surface to the center through internal circulation is well reflected in the new model, whereas the predictions by other models present a monotonic variation along the droplet's radius. They always underestimate the heating rate in the droplet's core region. However, the steady temperature of the droplet is unaffected by the choice of the liquid phase model.
- (2) The new 3rd-order model shows the best performance in predicting droplet evaporation during the later steady vaporizing period. The 2nd-order and conduction limit models significantly underestimate and overestimate the droplet evaporation rate in the case of *n*-Decane droplet exposed to a high temperature gas flow, respectively.
- (3) Although the 3rd- and 2nd-order models all derive from the lumped model with an identical energy equation, the former offers an important advantage in predicting both the temperature and evaporation evolution for moving droplets.
- (4) The new 3rd-order model has much higher computational efficiency than the conduction limit model and effective thermal conductivity model, with practical potential for their implementation into CFD codes.

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