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Two approaches to modelling the heating of evaporating droplets ☆

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ABSTRACT

Two approaches to modelling the heating of evaporating droplets have been widely used in engineering applications. In the first approach the heat rate supplied to the droplets to raise their temperatures, $\dot{q}_d$, is derived from the requirement that droplet evaporation rates, inferred from steady-state equations for mass and heat balance, should be the same. The second approach is based on the direct calculation of the distribution of temperature inside droplets assuming that their thermal conductivity is not infinitely large. The implications of these two approaches are compared for the case of stationary droplets in conditions relevant to Diesel engines. It is pointed out that although the trends of time evolution of $\dot{q}_d$ predicted by both approaches are similar, actual values of $\dot{q}_d$ predicted by these approaches can be visibly different. This difference can lead to noticeable differences in predicted droplet surface temperatures, radii and evaporation times. Possible reasons for these differences are discussed.

1. Introduction

Since the pioneering publications by Spalding (see [1]), the evaporation rate of stationary droplets $\dot{m}_d$ has been estimated based on the following well known equation [2,3]:

$$\dot{m}_d = -4\pi R_d D_v \rho_{\text{total}} \ln(1 + B_M), \qquad (1)$$

where

$$B_M = \frac{\rho_{vs} - \rho_{v\infty}}{\rho_{gs}} \qquad (2)$$

is the Spalding mass transfer number, ρ_{vs} and $\rho_v \infty$ are densities of vapour in the vicinity of droplet surfaces and at a large distance from them, ρ_g is the density of the ambient gas (air), R_d is the droplet radius, D_v is the diffusion coefficient of vapour in gas, and $\rho_{total} = \rho_g + \rho_v$ is the total density of the mixture of vapour and gas. Note that $\dot{m}_d \leq 0$.

The derivation of Expression (1) was based on a number of assumptions, perhaps one of the most important of which is the assumption that $\rho_{\text{total}} = $ const and does not depend on the distance from the droplet surface. This assumption can be justified when the temperature of the droplet is low and the difference between gas and droplet surface temperature is small (slow evaporation). In practical engineering applications, however, these restrictions of the range of applicability of Expression (1) are commonly ignored (e.g. [4]). Note that Expression (1)

cannot be used when the droplet surface temperature approaches boiling temperature when $\rho_{gs} = 0$ and B_M becomes infinitely large (e.g. [5]).

A more rigorous approach to the analysis of droplet evaporation was presented by Tonini and Cossali [6,7]. In the model suggested and developed in these papers, the requirement that $\rho_{\text{total}} = $ const was relaxed. The species, momentum and energy conservation equations were solved in a radial coordinate system, accounting explicitly for the gas density dependence on temperature and vapour concentration. However, as in the case of Expression (1), the problem was solved based on the quasi-steady state approximation (terms proportional to partial time derivatives were ignored in all equations) and the droplet surface temperature was assumed to be fixed during any time step. The effects of temperature gradient inside droplets were ignored (their thermal conductivity was assumed to be infinitely large).

An alternative expression for $\dot{m}_d$ was obtained based on the analysis of the heat balance equation. Assuming that the evaporating droplet is stationary, as in the case of Expression (1), this equation for an arbitrary distance $R > R_d$ from the centre of the droplet can be presented in the form [8]:

$$4\pi R^2 k_g \frac{dT}{dR} = -\dot{m}_d c_{pv}(T - T_s) - \dot{m}_d L(T_s) + \dot{q}_d, \qquad (3)$$

where k_g, c_{pv} and $L(T_s)$ are gas thermal conductivity, vapour specific heat capacity at constant pressure and specific heat of evaporation at the droplet surface temperature T_s. As in Expression (1), $\dot{m}_d \leq 0$. The left hand side of this equation shows the heat supplied from the surrounding gas to the droplet. The first term on the right hand side shows the heat required to heat fuel vapour from T_s to $T = T(R)$ (gas temperature

Nomenclature

B_M	Spalding mass transfer number
B_T	Spalding heat transfer number
c	specific heat capacity
D_v	binary diffusion coefficient of vapour in air
h	convection heat transfer coefficient
h_0	parameter introduced in Expression (9)
k	thermal conductivity
L	latent heat of evaporation
Le	Lewis number
$\dot{m}_d$	evaporation rate
$\dot{q}_d$	heat rate
q_n	parameter introduced in Expression (9)
R	distance from the droplet centre
R_d	droplet radius
t	time
T	temperature

Greek symbols

κ_R	parameter introduced in Expression (9)
λ	parameter defined by Eq. (10)
μ_0	parameter introduced in Expression (9)
ρ	density
φ	parameter defined by Eq. (7)

Subscripts

d	droplet
e	evaporation
eff	effective
g	gas
p	constant pressure
s	surface
v	vapour
∞	at a large distance from the droplet

at the distance R from the centre of the droplet). The second and third terms on the right hand side show the heat spent on droplet evaporation and raising its temperature (when $\dot{q}_d > 0$) respectively.

Rearranging this equation and its integration from $T = T_s$ to $T = T_g$ (ambient gas temperature) and from $R = R_d$ to $R = \infty$, assuming that the temperature dependence of k_g and c_{pv} can be ignored, gives [8]:

$$\dot{m}_d = -\frac{4\pi k_g R_d}{c_{pv}} \ln(1 + B_T), \qquad (4)$$

where

$$B_T = \frac{c_{pv}\left(T_g - T_s\right)}{L(T_s) - \left(\dot{q}_d / \dot{m}_d\right)} \qquad (5)$$

is the Spalding heat transfer number. From Eqs. (1) and (4) follows the relation between B_T and B_M [8]:

$$B_T = (1 + B_M)^\varphi - 1, \qquad (6)$$

where

$$\varphi = \left(\frac{c_{pv}}{c_{pg}}\right)\frac{1}{\text{Le}}, \qquad (7)$$

$\text{Le} = k_g/(c_{pg} D_{vg} \rho_{\text{total}})$ is the Lewis number.

Eq. (5) can be rewritten as:

$$\dot{q}_d = -\dot{m}_d \left[\frac{c_{pv}\left(T_g - T_s\right)}{B_T} - L(T_s)\right] = -\dot{m}_d \left[\frac{c_{pv}\left(T_g - T_s\right)}{(1 + B_M)^\varphi - 1} - L(T_s)\right]. \qquad (8)$$

Since the pioneering paper by Abramzon and Sirignano [8], Expression (8) has been widely used for modelling the heating of evaporating droplets. The assumptions on which the derivation of this expression was based (e.g. the validity of Expression (1)) have been almost universally ignored. An obvious limitation of Expression (8) is that the value of $\dot{q}_d$ is not affected by the thermal conductivity of liquid, which contradicts the physical nature of $\dot{q}_d$, as discussed later in the paper.

An alternative approach to the calculation of $\dot{q}_d$ could be based on the analysis of temperature distribution inside droplets, inferred from the direct analysis of convective heating of evaporating droplets (see [2] for the details). This approach is restricted to the case when liquid thermal conductivity is finite, which can be expected for any realistic liquid.

The focus of this paper is on the comparison of these two approaches to the calculation of $\dot{q}_d$ and their implications for the modelling of droplet heating and evaporation in conditions typical for Diesel engines. The analysis is focused on stationary droplets, although it can be easily generalised to the case of moving droplets, using the effective thermal conductivity (ETC) model (see [2,3]).

2. Model

Assuming that the convection heat transfer coefficient $h = \text{const}$, the solution to the heat conduction equation inside droplets, assuming that all processes are spherically symmetric, can be presented as [2,3]:

$$T(R, t) = \frac{R_d}{R} \sum_{n=1}^\infty \left\{ q_n \exp\left[-\kappa_R \lambda_n^2 t\right] - \frac{\sin\lambda_n}{||v_n||^2 \lambda_n^2}\mu_0(0)\exp\left[-\kappa_R \lambda_n^2 t\right] \right.$$
$$\left. - \frac{\sin\lambda_n}{||v_n||^2 \lambda_n^2}\int_0^t \frac{d\mu_0(\tau)}{d\tau}\exp\left[-\kappa_R \lambda_n^2(t-\tau)\right]d\tau \right\} \sin\left[\lambda_n\left(\frac{R}{R_d}\right)\right] + T_{\text{eff}}(t), \qquad (9)$$

where λ_n values are solutions to the equation:

$$\lambda\cos\lambda + h_0\sin\lambda = 0, \qquad (10)$$

$$||v_n||^2 = \frac{1}{2}\left(1 - \frac{\sin2\lambda_n}{2\lambda_n}\right) = \frac{1}{2}\left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right),$$
$$q_n = \frac{1}{R_d||v_n||^2}\int_0^{R_d}\widetilde{T}_0(R)\sin\left[\lambda_n\left(\frac{R}{R_d}\right)\right]dR, \quad \kappa_R = \frac{k_l}{c_l\rho_l R_d^2}, \quad \mu_0(t) = \frac{hT_g(t)R_d}{k_l},$$

$h_0 = (hR_d/k_l) - 1$ and $\widetilde{T}_0(R) = RT_{d0}(R)/R_d$. The solution to Eq. (10) gives a set of positive eigenvalues λ_n numbered in ascending order ($n = 1, 2, \ldots$),

$$T_{\text{eff}} = T_g + \frac{\rho_l L\dot{R}_{de}}{h}, \quad \dot{R}_{de} = \frac{\dot{m}_d}{4\pi R_d^2 \rho_l},$$

where ρ_l is the liquid density, and h for stationary evaporating droplets can be estimated as [2]:

$$h = \frac{2k_g}{R_d}\frac{\ln(1 + B_T)}{B_T}, \qquad (11)$$

where B_T is defined by Eq. (5).

The rate of droplet heating, leading to the rise of their temperatures, can be estimated as

$$\dot{q}_d = 4\pi R_d^2 k_l\frac{\partial T}{\partial R}\Big|_{R=R_d-0} \qquad (12)$$

where $\dot{q}_d > 0$ when the droplet is heated.

Having substituted (9) into (12) we obtain:

$$
\dot{q}_d = 4\pi R_d k_l \sum_{n=1}^{\infty} \left\{ q_n \exp\left[-\kappa_R \lambda_n^2 t\right] - \frac{\sin\lambda_n}{||v_n||^2 \lambda_n^2} \mu_0(0) \exp\left[-\kappa_R \lambda_n^2 t\right] \right.
$$
$$
\left. - \frac{\sin\lambda_n}{||v_n||^2 \lambda_n^2} \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp\left[-\kappa_R \lambda_n^2 (t-\tau)\right] d\tau \right\} [-1-h_0] \sin\lambda_n. \tag{13}
$$

Expression (13) is applicable to any time step with $t = 0$ referring to the beginning of the time step; t refers to the end of the time step. The values of $\dot{q}_d$ at the beginning of each time step are equal to the values of $\dot{q}_d$ at the end of the previous time step or the start of the heating process. Hence, without loss of generality we can assume that $t = 0$ in Expression (13). The values of $\dot{q}_d$ predicted by Expression (13) were shown to coincide within the accuracy of plotting with those predicted by Expression (12) using the numerical differentiation of the temperature predicted by Expression (9).

Expression (13) could be potentially generalised to take into account the effect of the moving droplet interface during the evaporation process, using the solution for the distribution of temperature inside a heated droplet presented in [9]. The analysis of the contribution of this effect, however, is beyond the scope of this paper.

Once the values of $\dot{q}_d$ have been obtained, the values of $\dot{m}_d$ can be obtained from the numerical solution of Eq. (4). The latter equation can be rewritten as:

$$
\dot{m}_d = -\frac{4\pi k_g R_d}{c_{pv}} \ln\left(1 + \frac{c_{pv}\left(T_g - T_s\right)\dot{m}_d}{L(T_s)\dot{m}_d - \dot{q}_d}\right). \tag{14}
$$

One can show that Eq. (14) has two solutions, $\dot{m}_d = 0$ (non-evaporating droplet) and $\dot{m}_d < 0$ (evaporating droplet), when

$$
\frac{4\pi k_g R_d\left(T_g - T_s\right)}{\dot{q}_d} > 1, \tag{15}
$$

and only one trivial solution $\dot{m}_d = 0$ (non-evaporating droplet) when Condition (15) is not satisfied.

In the limiting case when $B_T \ll 1$, Eq. (14) has the analytical solution:

$$
\dot{m}_d = \frac{1}{L(T_s)}\left[\dot{q}_d - 4\pi k_g R_d\left(T_g - T_s\right)\right]. \tag{16}
$$

This solution does not have physical meaning unless Condition (15) is satisfied. Expression (1) can still be used in this approach if

$$
B_M = (1 + B_T)^{1/\varphi} - 1. \tag{17}
$$

Eqs. (9), (11), (13) and (14) are applied at each time step. All thermodynamic and transport properties for liquid and gas are assumed constant during each time step but their changes from one time step to another due to the corresponding changes in temperature are taken into account. The effects of thermal swelling are taken into account using the conventional approach (see Eq. (25) of [4]).

3. Results and discussion

The model described in the previous section has been applied to the analysis of heating of an evaporating n-dodecane droplet in air at a pressure of 30 bar and temperature of 700 K. Thermodynamic and transport properties of n-dodecane are mainly taken to be the same as in [10], except for the diffusion coefficient for n-dodecane vapour in air which was taken from [11]. The initial droplet temperature and radius are assumed equal to 300 K and 10 μm respectively. The results predicted by Eqs. (13) and (14) (model 2) are compared with those predicted by the conventional model based on Expressions (1) and (8) (model 1). In both cases the finite thermal conductivity of liquid has been taken into

account and the distribution of temperature inside droplets has been predicted by Eq. (9).

The values of $\dot{q}_d$, predicted by these two approaches are shown in Fig. 1. Note that at the very final stages of droplet evaporation the values of $\dot{q}_d$ predicted by the model based on Eqs. (13) and (14) became negative (although close to zero) which eventually led to the situation when Eq. (14) had no real solutions. To avoid this situation the distribution of temperature inside droplets was frozen at the moment when $\dot{q}_d = 0$. Also, at the very final stage of droplet evaporation, the predicted droplet temperature could approach the critical temperature and even exceed it. This was partly remedied by assuming that once T_{eff} has reached its minimal value it remains at this level until the droplet fully evaporates. These assumptions are expected to produce minor effects on the predicted surface temperatures and radii of droplets which are not important for practical applications. The problems with modelling droplet heating and evaporation at the final stages of droplet evaporation when $dR_d/dt \rightarrow \infty$ were recognised in our previous studies (e.g. [12]).

As one can see from Fig. 1, the time dependence trends for $\dot{q}_d$, predicted by both approaches are rather similar, but the actual values of $\dot{q}_d$ are noticeably different. This difference in the values of $\dot{q}_d$ leads to rather large differences in the corresponding values of droplet radii and surface temperatures versus time, as shown in Fig. 2. As follows from the latter figure, the model based on Eqs. (13) and (14) predicts lower droplet surface temperatures and shorter evaporation times compared with the model based on Expressions (1) and (8). Lower droplet surface temperatures predicted by model 2 compared with model 1 are expected to lead to lower values of the heat fluxes at the surface of the droplet. This is consistent with the predicted values of $\dot{q}_d$ shown in Fig. 1.

Similar trends in time evolution of the parameters predicted by both models allow us to use them for qualitative analysis of droplet evaporation, but their reliability for quantitative analysis of the processes remains unclear. One of the reasons for the differences between the predicted results might lie in the fact that both approaches to the calculation of the evaporation rate are based on the quasi-steady-state approximation. The limitations of this approximation for the case of non-evaporating droplet heating were discussed in [13,14].

4. Conclusions

Two approaches to modelling the heating of evaporating droplets have been compared. In the first approach, the heat rate supplied to the droplets to raise their temperatures, $\dot{q}_d$, is derived from the requirement that the rates of droplet evaporation $\dot{m}_d$, inferred from steady-state equations for mass and heat balance in the gas phase, should be the same (in this approach the values of $\dot{q}_d$ do not depend on the value of
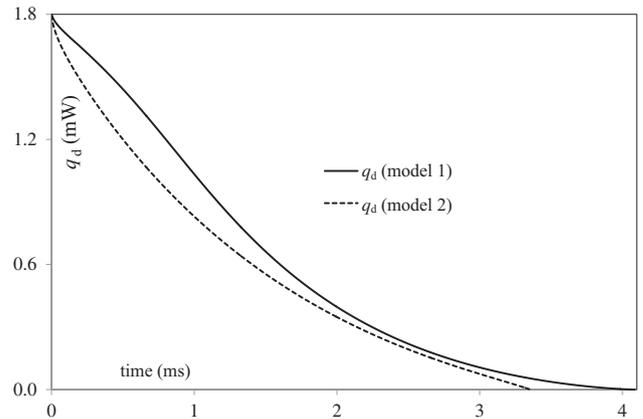

Fig. 1. Plots of $\dot{q}_d$ versus time predicted by the model based on Expressions (1) and (8) (model 1) and Eqs. (13) and (14) (model 2) for an evaporating n-dodecane droplet heated in air at a pressure of 30 bar and temperature of 700 K. The initial droplet temperature and radius are assumed to be equal to 300 K and 10 μm respectively.
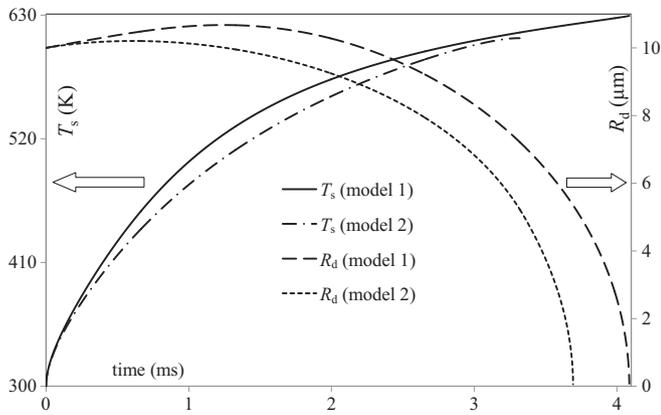
Fig. 2. The same as in Fig. 1 but for droplet surface temperatures (T_s) and radii (R_d).

liquid thermal conductivity). The second approach is based on the direct calculation of the distribution of temperature inside droplets assuming that their thermal conductivity is not infinitely large. The implications of these two approaches are compared for the case of stationary droplets in conditions relevant to Diesel engines. It is pointed out that the trends in $\dot{q}_d$ time evolution, predicted by both approaches, are similar, but the actual values of $\dot{q}_d$ at any given time instant are visibly different. This difference can lead to noticeable differences in predicted droplet surface temperatures, radii and evaporation times. One possible reason for these differences is that the calculations of the evaporation rate in both approaches are based on the quasi-steady-state approximation. It is concluded that both approaches to the calculation of $\dot{q}_d$ can be applied for qualitative analysis of droplet heating and evaporation, but caution should be exercised when using either of them for quantitative analysis.

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