Modelling of droplet heating and evaporation: recent results and unsolved problems

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Abstract. The most recent results referring to the hydrodynamic and kinetic modelling of droplet heating and evaporation are briefly summarised. Two new solutions to the heat conduction equation, taking into account the effect of the moving boundary during transient heating of an evaporating droplet, are discussed. The first solution is the explicit analytical solution to this equation, while the second one reduces the solution of the differential transient heat conduction equation to the solution of the Volterra integral equation of the second kind. It has been pointed out that the new approach predicts lower droplet surface temperatures and slower evaporation rates compared with the traditional approach. A simplified model for multi-component droplet heating and evaporation, based on the analytical solution of the species diffusion equation inside droplets, is reviewed. A new algorithm, based on simple approximations of the kinetic results for droplet radii and temperatures, suitable for engineering applications, is discussed.

1. Introduction
The importance of accurate and CPU efficient modelling of droplet heating and evaporation in various engineering and environmental applications is well recognised. These models are typically based on a number of rather restrictive assumptions, including the assumption that the thermal conductivity of droplets is infinitely large and, in the case of multi-component droplets, the diffusivity of species within them is infinitely large or small. Kinetic effects have been ignored. In a series of our previous papers, a number of simplified models of droplet heating and evaporation have been developed, where the effects of the finite thermal conductivity of droplets and recirculation within them, and kinetic effects in the evaporation process have been taken into account \cite{1}-\cite{6}. The format of most of these models was such that they could be incorporated into CFD codes and used for modelling real-life engineering processes. The results of these papers are summarised in a number of reviews, including \cite{7}-\cite{9}.

The aim of this paper is to summarise some results of the most recent developments of these models. These new or further developed models take into account the impact of moving boundary and kinetic effects on the evaporation process and the finite rate of species diffusion in multi-component droplets. The models are presented in the format in which they can be potentially implemented into engineering CFD codes. This review is essentially an updated
version of the previous review [9]. Particular emphasis is put on unsolved problems on which we are currently working.

2. Effects of the moving boundary
The models for droplet heating used in [1, 2] were implicitly based on the assumptions that the evaporation rate of droplets is small and the value of droplet radius $R_d$ does not change during any time step (although this radius changes from one step to another). This means that the effect of a moving boundary on droplet heating was ignored. This is a well known approach used in all available CFD codes. We attempted to take into account the changes in droplet radius $R_d$ during the time steps. Two approaches were developed. Firstly it was assumed that $R_d$ is a linear function of time. Secondly, we calculated the evolution of droplet temperature for an \textit{a priori} fixed function $R_d(t)$. In both cases the droplet temperature ($T \equiv T(t, R)$) was found from the solution of the heat conduction equation in the form [10, 11]:

$$\frac{\partial T}{\partial t} = \kappa \left( \frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right)$$

for $0 \leq t < t_e$, $0 \leq R < R_d(t)$, where $\kappa$ is the liquid thermal diffusivity ($\kappa = k_l/(c_l \rho_l)$), $k_l$ is the thermal conductivity, $c_l$ is the specific heat capacity, $\rho_l$ is the density, $R$ is the distance from the centre of the droplet. The effect of thermal radiation is ignored.

Remembering the physical background to the problem, we look for the solution of this equation in the form of a twice continuously differentiable function $T \equiv T(t, R)$ for $0 \leq t < t_e$, $0 \leq R < R_d(t)$. This solution should satisfy the boundary condition:

$$\left( k_l \frac{\partial T}{\partial R} + hT \right)_{R=R_d(t)} = hT_g + \rho_l L \dot{R}_d(t),$$

where $T$ is finite and continuous at $R \to 0$, $T_s = T(R_d(t), t)$ is the droplet’s surface temperature, $L$ is the latent heat of evaporation. We took into account that $\dot{R}_d(t) \equiv dR_d/dt \leq 0$. Effects of swelling are ignored. Equation (2) is the energy balance condition at $R = R_d(t)$. The initial condition is taken in the form:

$$T(t = 0) = T_0(R),$$

where $0 \leq R \leq R_{d0} = R_d(t = 0)$. The value of $R_d(t)$ is controlled by fuel vapour diffusion from the droplet surface, and can be found from the equation [7]:

$$\dot{R}_d = \frac{-k_g \ln (1 + B_M)}{\rho_l c_{pg} R_d},$$

where $B_M = Y_{vs}/(1 - Y_{vs})$ is the Spalding mass transfer number, $Y_{vs}$ is the mass fraction of fuel vapour near the droplet surface, which is ultimately controlled by gas temperature [7].

In the model described in [1, 2], equation (1) with the boundary condition (2) and fixed $R_d$ and $h$ during the time step was solved analytically. This solution was used for the determination of the distribution of temperature inside droplets at the end of the time step. The value of $R_d$ at the end of this time step was obtained from equation (4). The distribution of temperature at the beginning of the next time step was recalculated for the new droplet radius. This model was generalised by assuming that $R_d(t)$ is the linear function of $t$ during the time step [12]:

$$R_d(t) = R_{d0}(1 + \alpha t).$$

Remembering (4), the expression for $\alpha$ can be presented as:

$$\alpha = -\frac{k_g \ln (1 + B_M)}{\rho_l c_{pg} R_{d0}^2}.$$
Assuming that $\alpha$ (rather than $R_d$) is fixed during the time step, the analytical solution to equation (1) subject to the above boundary and initial conditions was obtained in the form [12]

$$T(R) = \frac{1}{R \sqrt{R_d(t)}} \exp \left[ -\frac{\alpha R_d(t) R^2}{4\kappa R_d(t)} \right] = \left[ \sum_{n=1}^{\infty} \Theta_n(t) \sin \left( \lambda_n \frac{R}{R_d(t)} \right) + \mu_0(t) \frac{R}{1 + h_0 R_d(t)} \right],$$  \hspace{1cm} (7)

where

$$\Theta_n(t) = \Theta_n(0) \exp \left[ \frac{\kappa \lambda_n^2}{\alpha R^2_{d0}} \left( \frac{1}{1 + \alpha t} - 1 \right) \right] + f_n \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp \left[ \frac{\kappa \lambda_n^2}{\alpha R^2_{d0}} \left( \frac{1}{1 + \alpha t} - \frac{1}{1 + \alpha \tau} \right) \right] d\tau,$$

$$\mu_0(t) = \tilde{\mu}(t) \sqrt{R_d(t)} \exp \left[ \frac{R_d'(t) R_d(t)}{4\kappa} \right], \hspace{1cm} (8)$$

$$\tilde{\mu}(t) = M(t) R^3_{d0}(t), \hspace{0.5cm} M(t) = \frac{h}{k_l} T_n + \frac{\rho_0 L R(t)}{k_l}, \hspace{0.5cm} f_n = -\frac{\sin \lambda_n}{||v_n|| \xi_n^2}, \hspace{0.5cm} v_n(\xi) = \sin \lambda_n \xi \hspace{0.5cm} (n = 1, 2, ...).$$

$$||v_n||^2 = \frac{1}{2} \left( 1 - \frac{\sin 2\lambda_n}{2\lambda_n} \right) = \frac{1}{2} \left( 1 + \frac{h_0}{h_0^2 + \lambda_n^2} \right).$$  \hspace{1cm} (9)

$\lambda_n$ are positive solutions to the equation

$$\lambda \cos \lambda + h_0 \sin \lambda = 0$$  \hspace{1cm} (10)

presented in ascending order,

$$h_0 = \frac{h(t)}{k_l} R_d(t) - 1 - \frac{R_d'(t) R_d(t)}{2\kappa}$$  \hspace{1cm} (11)

is assumed to be constant during the time step,

$$\Theta_n(0) = q_n + \mu_0(0) f_n, \hspace{0.5cm} q_n = \frac{1}{||v_n||^2} \int_0^1 W_0(\xi) v_n(\xi) d\xi.$$

$$W_0(\xi) = R^{3/2}_{d0} T_0(\xi R_{d0}) \exp \left[ \frac{R_d(0) R_{d0}}{4\kappa \xi} \right].$$  \hspace{1cm} (12)

If Assumption (5) is replaced by the assumption that $T_{d0}(R) = \text{const}$ then the solution of equation (1) subject to the above-mentioned boundary and initial conditions can be presented as:

$$T(t, R) = T_{d0} + \frac{\sqrt{\kappa}}{2R \sqrt{\pi}} \int_0^t \frac{\nu(\tau)}{\sqrt{t - \tau}} \left\{ \exp \left[ -\frac{(R - R_d(\tau))^2}{4\kappa(t - \tau)} \right] - \exp \left[ -\frac{(R + R_d(\tau))^2}{4\kappa(t - \tau)} \right] \right\} d\tau, \hspace{1cm} (13)$$

where $\nu(\tau)$ is the solution to the following integral equation:

$$\frac{\nu(t)}{2} + \int_0^t \frac{\nu(\tau)}{\sqrt{t - \tau}} \left\{ \frac{\partial G(t, \tau, R)}{\partial R} \bigg|_{R=R_d(t)} + H(t) G(t, \tau, R_d(t)) \right\} d\tau = \mu_0(t), \hspace{1cm} (14)$$

where

$$G(t, \tau, R) = \frac{\sqrt{\kappa}}{2 \sqrt{\pi(t - \tau)}} \left\{ \exp \left[ -\frac{(R - R_d(\tau))^2}{4\kappa(t - \tau)} \right] - \exp \left[ -\frac{(R + R_d(\tau))^2}{4\kappa(t - \tau)} \right] \right\}$$  \hspace{1cm} (15)

$$\nu(t) = \frac{\sqrt{\kappa}}{2 \sqrt{\pi(t - \tau)}} \left\{ \exp \left[ -\frac{(R - R_d(\tau))^2}{4\kappa(t - \tau)} \right] - \exp \left[ -\frac{(R + R_d(\tau))^2}{4\kappa(t - \tau)} \right] \right\}$$  \hspace{1cm} (16)
calculations were performed for $R_f$ droplets [7]:

\[ m(T) = \frac{\rho_m}{k_f} \frac{\partial T}{\partial t} + \frac{\mu_t}{k_t} R_d(t) T_{db} + \mu(t), \]

\[ M(t) = \frac{\rho_m}{k_f} T_g + \frac{\mu_t}{k_t} L \dot{R}_d(t). \]

Solution (14) was applied iteratively. At first $R_d(t)$ was found using the conventional approach when $R_d = \text{const}$ during the time step. Then this $R_d(t)$ was substituted into Solution (14). At the next step this solution for $T(R, t)$ was used to obtain the updated value of $R_d(t)$ etc. The calculations were performed for $R_{db} = 10 \ \mu m$, and gas temperature was taken equal to 1000 K. We assumed that fuel can be approximated as n-dodecane ($M_f = 170 \ \text{kg/kmole}$) and $p = 3000 \ \text{kPa}$ (typical values for Diesel engine-like conditions). The time step 0.008 ms was used for the conventional approach while the time step 0.01 ms was used for the new approach based on Solution (7). The predictions of Solutions (7) and (14) practically coincided which gives additional confidence in our new model. The new approach predicts slightly smaller droplet surface temperatures and slightly longer evaporation times compared with the conventional approach ($t_{e(\text{new})} - t_{e(\text{conventional})})/t_{e(\text{new})} = (2.49 \ \text{ms} - 2.38 \ \text{ms}) / 2.49 \ \text{ms} = 0.044 = 4.4\%$). This increase in the evaporation time is certainly large enough to warrant taking into account the effect considered in this paper in the practical modelling of droplet heating and evaporation for engineering applications.

### Species diffusion inside droplets

The analysis will be restricted to the models of multi-component droplet heating and evaporation based on the analysis of individual components (e.g. [13, 14, 15]), applicable in the case when a small number of components needs to be taken into account. Moreover, at this stage only the simplest case of bi-component droplets is considered, as in [15], which allows us to develop a better understanding of the underlying physics of the processes involved. The new model, originally described in [16, 17], is much simpler than the vortex models (e.g. [15]) which makes it potentially attractive for implementation into computational fluid dynamics (CFD) codes. The predictions of the model agreed with the measured time evolution of droplet temperatures in monodisperse bi-component (ethanol/acetone) droplet streams.

The new model is based on the analytical solution (7) for $R_d = \text{const}$ combined with equation (4) as in the case of the mono-component droplets considered in the previous section. These equations are complemented by the equation for species mass fraction ($Y_{li} \equiv Y_{li}(t, R)$) inside droplets [7]:

\[ \frac{\partial Y_{li}}{\partial t} = D_l \left( \frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right), \]  

(17)

where $i = 1, 2$, $D_l$ is the liquid mass diffusivity. Equation (17) is solved with the following boundary condition [7]:

\[ \alpha_Y \left( \epsilon_i - Y_{lis} \right) = -D_l \left. \frac{\partial Y_{li}}{\partial R} \right|_{R=R_d-0} , \]  

(18)

and the initial conditions $Y_{li}(t = 0) = Y_{li0}(R)$, where $Y_{li} = Y_{lis}(t)$ are liquid components’ mass fractions at the droplet’s surface,

\[ \alpha_Y = |\dot{m}_d| / \left( 4\pi \rho R_d^2 \right), \]  

(19)

$\dot{m}_d$ is the droplet evaporation rate determined by equation (4), $\epsilon_i$ are species evaporation rates determined from the following equation:

\[ \epsilon_i = Y_{visi} \sum Y_{vis}, \]  

(20)

where the subscript $v$ indicates the vapour phase.
Equations (1) and (17), originally derived for spherically symmetric stationary droplets, were
generalised to the case of moving droplets by replacing \( k_l \) and \( D_l \) with the so called
effective thermal conductivity and diffusivity \[7, 18\]:

\[
k_{\text{eff}} = \chi k_l, \quad D_{\text{eff}} = \chi Y D_l,
\]

where the coefficients \( \chi \) and \( \chi Y \) vary from 1 to 2.72 depending on Reynolds, Prandtle
and Schmidt numbers (see \[7\] for details); in the case of stationary droplets \( \chi = \chi Y = 1 \).

The molar fractions of species \( i \) in the vapour phase at the surface of the droplet were
determined from the following equation:

\[
X_{vi} = X_{li} \gamma_i \exp \left[ \frac{L_i M_i}{R_u} \left( \frac{1}{T_{bi}} - \frac{1}{T_s} \right) \right],
\]

(21)

where \( X_{li} \) is the liquid molar fraction at the surface of the droplet, \( \gamma_i \) is the activity
coefficient, \( L_i M_i \) and \( T_{bi} \) are the latent heat of evaporation, molar mass and boiling temperature of species
\( i \) respectively, \( R_u \) is the universal gas constant, \( T_s \) is the droplet surface temperature. The
activity coefficient for the ethanol-acetone mixture was estimated following \[19\].

Although equation (17) looks identical to (1), Solution (5) to equation (1) cannot be used
for equation (17), due to different boundary conditions (equations (2) and (19)). The analytical
solution to equation (17), subject to the above boundary and initial conditions was obtained in
the form \[16, 17\]:

\[
Y_{li} = \epsilon_i + \frac{1}{R} \left\{ \exp \left[ D_l \left( \frac{\lambda_0}{R_d} \right)^2 t \right] \left[ q_{i0} - \epsilon_i(0)Q_0 \right] \right\} \sinh \left( \frac{\lambda_0 R}{R_d} \right)
+ \sum_{n=1}^{\infty} \left\{ \exp \left[ -D_l \left( \frac{\lambda_n}{R_d} \right)^2 t \right] \left[ q_{in} - \epsilon_i(0)Q_n \right] \right\} \sin \left( \frac{\lambda_n R}{R_d} \right),
\]

(22)

where

\[
Q_n = \begin{cases}
-\frac{1}{||v_0||^2} \left( \frac{R_d}{\lambda_0} \right)^2 (1 + h_0) \sinh \lambda_0 & \text{when } n = 0 \\
\frac{1}{||v_n||^2} \left( \frac{R_d}{\lambda_n} \right)^2 (1 + h_0) \sin \lambda_n & \text{when } n \geq 1
\end{cases}
\]

(23)

\[
q_{in} = \frac{1}{||v_n||^2} \int_0^{R_d} R Y_{li0}(R) v_n(R) dR,
\]

(24)

\( n \geq 0, \lambda_0 \) is the solution to the equation

\[
\tanh \lambda = -\frac{\lambda}{h_0},
\]

(25)

while \( \lambda_n (n \geq 1) \) are solutions to equation (11),

\[
h_0 = -\left( 1 + \frac{\alpha R_d}{D_l} \right),
\]

(26)

(note that \( h_0 \) used in this section is different from the one used in the previous section; the same
symbol is used in both cases to highlight similarities between two solutions),

\[
v_n = \begin{cases}
\sinh \left( \frac{\lambda_0 R}{R_0} \right) & \text{when } n = 0 \\
\sin \left( \frac{\lambda_n R}{R_0} \right) & \text{when } n \geq 1
\end{cases}
\]

(27)

Solution (22) was incorporated into the numerical scheme for simulating monodisperse
ethanol-acetone droplet heating and evaporation in the experiment described in \[15\]. The
results referring to average droplet temperatures were shown to be reasonably close to both
experimental data and the predictions of the more rigorous and complex vortex model. This
could justify the application of this model instead of the vortex model for modelling the processes
of multi-component droplet heating and evaporation.
3. Kinetic effects
In a series of our previous papers (see [5] and the references therein) it was demonstrated that, even in the case of droplet heating and evaporation into a high-pressure gas (Diesel engine-like conditions), the kinetic effects may not be negligible. In these papers, two regions of gas above the surface of the evaporating droplet were considered: the kinetic and hydrodynamic regions. In the most comprehensive model, described in [5], it was assumed that gas consisted of two components, fuel vapour and background gas (air), and both mass and heat transfer processes in the kinetic region were taken into account. The analysis of the processes in this region was based on the numerical solution of the Boltzmann equations for fuel vapour and background gas with the relevant boundary conditions. The CPU requirements of this solution, however, make it impossible to incorporate it into engineering computational fluid dynamics (CFD) codes designed to model fuel droplet evaporation in a realistic engineering environment, taking into account all complexities of the processes in Diesel engines (see [20, 21]).

It seems the only feasible way to apply the results of [5] to the analysis of Diesel fuel droplet heating and evaporation within these CFD codes would be to approximate the results of kinetic calculations using simple approximate analytical formulae. The selection of the approximations should be based on finding a compromise between their accuracy and simplicity. The preliminary results of our analysis in this direction were reported in [22, 23]. Some more recent results are presented in this section, based on [6, 9]. The most important ranges of the values of fuel droplet radii and gas temperatures were considered, while the initial value of droplet temperature was assumed equal to 300 K. Although the applicability of the approximations found was restricted to the very specific problem of modelling the processes in Diesel engines, it is anticipated that this approach can be generalised to a much wider range of engineering applications.

Based on the direct comparison of the results of kinetic and hydrodynamic computations for gas temperatures $T_g=750$ K, 1000 K and 1500 K and initial droplet radii $R_0=5$ µm and $R_0=20$ µm, it was shown that the best approximation for droplet radii, predicted by the kinetic model, can be achieved using the following formula:

$$
\Delta R = a_{1R} \exp\left(-\frac{R}{t_{1R}}\right) + a_{2R} \exp\left(-\frac{R}{t_{2R}}\right),
$$

where

$$
\Delta R = (R_{dk} - R_{dh}) / R_{d0}, \quad \bar{R} = R_{dh} / R_{d0},
$$

$R_{dk}$ and $R_{dh}$ are droplet radii predicted by the kinetic and hydrodynamic models respectively, $R_{d0}$ is the initial droplet radius, the coefficients $a_{1R}$, $a_{2R}$, $t_{1R}$ and $t_{2R}$ are fitting constants. The effects of droplets on gas temperature were ignored, following [5].

A slightly less accurate, but simpler approximation was found in the form:

$$
\Delta R = a_{3R} \exp\left(-\frac{R}{t_{3R}}\right),
$$

where $a_{3R}$ and $t_{3R}$ are new fitting constants.

All these fitting constants are presented in [6, 9] for several combinations of initial droplet radii and gas temperatures. As follows from our analysis, the first approximation is almost ideal, while there are some noticeable deviations between the predictions of Formula (29) and the results of calculations. These deviations can be ignored in many practical applications. Similar closeness between the results of calculations and approximations was demonstrated for other combinations of $R_{d0}$ and $T_g$ considered above. Approximations (28) and (29) can be interpolated for the whole range of gas temperatures from 750 K to 1500 K, using the following
interpolation formula for the coefficients $a_{1R}$, $a_{2R}$, $t_{1R}$ and $t_{2R}$ (we restricted this interpolation to Approximation (28) only):

$$s_R = b_{0R} + b_{1R} \tilde{T} + b_{2R} \tilde{T}^2,$$

(30)

where $\tilde{T} = T_g/T_{cr}$, $T_{cr} = 659$ K is the critical temperature of n-dodecane C$_{12}$H$_{26}$ (approximation of Diesel fuel), $s_R$ stands for $a_{1R}$, $a_{2R}$, $t_{1R}$ or $t_{2R}$. The values of coefficients $b_{iR}$, where $i = 0$, 1, 2, for $R_{d0} = 20$ $\mu$m and $R_{d0} = 5$ $\mu$m are given in [6, 9]. The values of coefficients $a_{1R}$, $a_{2R}$, $t_{1R}$ and $t_{2R}$, predicted by Approximation (30) for $R_{d0} = 20$ $\mu$m and $R_{d0} = 5$ $\mu$m and $T_g = 750$ K, 1000 K and 1500 K are also given in [6, 9]. The maximal difference between the values of fitting constants did not exceed about 1%. This justifies the application of Approximation (30).

Based on the direct comparison of the results of kinetic and hydrodynamic calculations for the same gas temperatures and initial droplet radii as in the previous section, we were able to show that a good approximation for the droplet temperatures predicted by the kinetic model can be achieved using the following formula:

$$\Delta T = a_{1T} \exp \left(-\frac{T}{t_{1T}}\right) + a_{2T},$$

(31)

where

$$\Delta T = \frac{T_h - T_0}{T_{cr} - T_0}, \quad \tilde{T} = \frac{T_h - T_0}{T_{cr} - T_0}.$$

$T_k$ and $T_h$ are droplet temperatures predicted by the kinetic and hydrodynamic models respectively, $T_0$ is the initial droplet temperature, the coefficients $a_{1T}$, $t_{1T}$ and $a_{2T}$ are fitting constants. These constants are presented in [6, 9] for the same combinations of initial droplet radii and gas temperatures as in the previous section.

The closeness of the plots of $\Delta T = \frac{T_k - T_h}{T_{cr} - T_0}$ versus $T = \frac{T_h - T_0}{T_{cr} - T_0}$ obtained using the kinetic model (calculation) and approximate equation (31) was demonstrated for various combinations of $R_{d0}$ and $T_g$ considered above.

As in the case of droplet radii, Approximation (31) with the values of coefficients given in [6, 9], can be interpolated for the whole range of gas temperatures from 750 K to 1500 K, using Approximation (30) for the coefficients $a_{1T}$, $a_{2T}$ and $t_{1T}$, replacing subscript $R$ with $T$ everywhere. As a result, equation (30) is replaced by:

$$s_T = b_{0T} + b_{1T} \tilde{T} + b_{2T} \tilde{T}^2,$$

(32)

where $s_T$ stands for $a_{1T}$, $a_{2T}$ or $t_{1T}$. The values of these coefficients are given in [6, 9].

The values of coefficients $a_{1T}$, $t_{1T}$ and $a_{2T}$, predicted by Approximation (32) for $R_{d0} = 20$ $\mu$m and $R_{d0} = 5$ $\mu$m, and for $T_g = 750$ K, 1000 K and 1500 K are given in [6, 9]. The maximal difference between the values of fitting constants did not exceed about 1%. This justifies the application of Approximation (32).

4. Conclusions
Recently developed approaches to the hydrodynamic and kinetic modelling of fuel droplet heating and evaporation are reviewed. Two new solutions to the heat conduction equation, describing transient heating of an evaporating droplet, are discussed. The first solution is the explicit analytical solution to this equation, while the second one reduces the solution of the differential transient heat conduction equation to the solution of the Volterra integral equation of the second kind. Both solutions take into account the effect of the reduction of the droplet radius due to evaporation. It is anticipated that the analytical solution can be used in computational fluid dynamics (CFD) codes to describe droplet heating and evaporation over a small time step when all parameters, except droplet radius and temperature, can be assumed constant. This can
be considered as the generalisation of the approach currently used in all research and commercial CFD codes, in which it is assumed that droplet radius is constant during the time step. It has been pointed out that the new approach predicts lower droplet surface temperatures and slower evaporation rates compared with the traditional one.

A simplified model for bi-component droplet heating and evaporation is developed and applied for the analysis of the observed average droplet temperatures in a monodisperse spray. The model takes into account all key processes, which take place during this heating and evaporation, including the distribution of temperature and diffusion of liquid species inside the droplet and the effects of the non-unity activity coefficient (ideal and non-ideal models). The effects of recirculation in the moving droplets on heat and mass diffusion within them are taken into account using the effective thermal conductivity and the effective diffusivity models. The previously obtained analytical solution of the transient heat conduction equation inside droplets is incorporated in the numerical code alongside the original analytical solution of the species diffusion equation inside droplets.

A new algorithm, based on simple approximations of the kinetic results for droplet radii and temperatures, suitable for engineering applications, is discussed. These approximations are based on the presentation of the kinetic effects as corrections to the results of the hydrodynamic calculations. These corrections are presented in the form of simple algebraic expressions. The analysis described is applicable to a wide range of problems related to droplet heating and evaporation, although the main emphasis is on the application to Diesel engines.

5. Unsolved problems
The complete list of unsolved problems, referring to droplet heating and evaporation, is open-ended. In what follows we will restrict ourselves to the problems on which we are currently working.

5.1. Combined model, taking into account the effects of moving boundary, multi-component droplets and thermal radiation
The models described in Sections 2 and 3 took into account either the effects of a moving boundary, or the effects of multi-component droplets, but not a combination of the two. Also, at this stage, the contribution of thermal radiation was not taken into account (cf. the original model described in [1]). We are currently working on the model in which all these effects are taken into account simultaneously.

5.2. Effects of non-elastic collisions in the kinetic model
One of the most important limitations of the kinetic model described in Section 3, is that it is based on the assumption that collisions between molecules are elastic. This could be acceptable in the case of mono-atomic molecules (e.g. Argon). However, in the case of complex hydrocarbons, such as n-dodecane (approximation of Diesel fuel) it is not at first obvious that the contribution of internal degrees of freedom can be ignored. We are currently working on the development of a new model for inelastic collisions which would be simple enough to take into account the effect of such collisions in the kinetic model.

5.3. Evaporation coefficient of complex hydrocarbons
One of the parameters of the kinetic model is the evaporation coefficient of molecules at the surface of the droplets. Possible approaches to experimental measurements of this coefficient
and its crude estimates are discussed in our previous papers (e.g. [7, 22]). The most accurate estimate of this coefficient should be based on molecular dynamics (MD) simulations. MD technique is reasonably well developed for relatively simple molecules, but nobody, to the best of our knowledge, has attempted to apply this technique to complex hydrocarbon molecules, such as n-dodecane. At the moment we are in the process of developing such a technique and are working on its application to calculation of the evaporation coefficient of n-dodecane droplets.

5.4. Approximation of the results of kinetic calculations using simple formulae

Once the developments of the kinetic model, described above, have been completed, the results of kinetic calculations would need to be approximated by simple formulae, similar to those described in Section 4. This would enable us to incorporate these approximations into computational fluid dynamic (CFD) codes and use them in various engineering and environmental applications.

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