A kinetic algorithm for modelling the droplet evaporation process in the presence of heat flux and background gas

S. S. Sazhin\textsuperscript{\textcopyright,1}, I. N. Shishkova\textsuperscript{*}

\textsuperscript{\textcopyright}Sir Harry Ricardo Laboratories, School of Environment and Technology, University of Brighton, Cockcroft Building, Brighton BN2 4GJ, U.K.

*Low Temperature Department, Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

\textsuperscript{1}Corresponding author, e-mail: S.Sazhin@brighton.ac.uk

To be published in ‘Atomization and Sprays’ June 14, 2008

Keywords: Boltzmann equation, Diesel fuel, fuel droplets, heating, evaporation

Abstract

A kinetic model for droplet heating and evaporation into a high pressure background gas (air) is described. This model is based on the introduction of the kinetic region around evaporating droplets, where the dynamics of molecules are described in terms of the Boltzmann equations for vapour and air. Both mass and heat transfer processes in this region are taken into account. The conditions at the outer boundary of the kinetic region are introduced by matching the mass fluxes of vapour leaving the kinetic region and entering into the surrounding hydrodynamic region, and the corresponding heat fluxes. The new model is applied to calculations of heating and evaporation of fuel droplets in Diesel engine-like conditions. It is pointed out that in the case of droplet heating in a relatively cool gas ($T_g = 750$ K), the effect of non-zero heat flux in the kinetic region is negligible. This effect, however, turns out to be important in the cases where gas temperature rises to 1000 K and 1500 K. In the latter case, for droplets with initial radii equal to 5 $\mu$m the predicted evaporation time in the presence of the heat flux in the kinetic region proves to be about 14% longer than predicted by the hydrodynamic model. The increase in this time in the case where the heat flux in the kinetic region is ignored would only be about 8%. The application of the rigorous kinetic model, taking into account the heat flux in the kinetic region, as described in this paper, is recommended when accurate predictions of the values of droplet surface temperature and evaporation time are essential.
1 Introduction

The applications of kinetic methods to the modelling of evaporation, condensation and other transfer processes have been described in numerous publications (e.g. [1]-[8]). Although these methods have been almost exclusively applied to the cases when gases are rarefied with Knudsen numbers (Kn) exceeding $10^{-2}$, a number of authors have drawn attention to the fact that, even in the case where Kn \rightarrow 0, the application of hydrodynamic methods to modelling fluid dynamics and heat and mass transfer processes is not always justified [9]-[14]. In the recent paper by Kryukov et al [12] it was demonstrated that, even in the case of droplet evaporation into high pressure (30 bar) gas (Diesel engine-like conditions), the kinetic effects may not be negligible. It was shown that these effects can lead to increases in the evaporation time by up to 5-10\%, compared with the prediction of the conventional hydrodynamic model in the case of small droplets (radii about 5 \textmu m) injected into a hot gas with temperatures $T_g = 750$-2000 K. The model used in [12] was based on the approximate analysis of the Boltzmann equation, performed under a number of assumptions (e.g. a small Knudsen number, the gas temperature close to the droplet surface temperature, the collisional term in the Boltzmann equation taken in the form suggested by Bhatnagar, et al [15]) and leading to an explicit expression for mass flux of vapour leaving the droplet. Two of these assumptions seem to be particularly important for practical applications. These are the assumption that the evaporation coefficient $\beta$ is a priori given and the assumption that no other gases, apart from vapour, are present in the vicinity of the droplet surface. The evaporation coefficient is defined as the ratio of the actual mass flux leaving the surface of the droplet $j_{es}$ (before the first collision between fuel vapour molecules leaving the droplet surface and vapour and air molecules present in the kinetic region) and the maximal possible mass flux:

$$\beta = \frac{j_{es}}{\rho_{vs} \sqrt{\frac{R_v T_s}{2\pi}}},$$

where $\rho_{vs}$ is the density of saturated fuel vapour corresponding to the liquid temperature at the droplet surface, $T_s = T_{ls}$, $R_v$ is the gas constant for fuel vapour. Since no direct measurements or calculations of $\beta$ for Diesel fuel were available when paper [12] was prepared, the minimal and average values of this parameter for water (0.04 and 0.5) were used. The second assumption can hardly be justified in the case of Diesel fuel droplet evaporation into high pressure air [16, 17].

A number of authors considered the problem of the evaporation and condensation of liquid droplets in the presence of inert gas based on simplified kinetic models. For example, Onishi [18] based his analysis on the linearised Boltzmann equation of the Bhatnagar-Gross-Krook type [15] (see [19]), while the analysis by Young [20] ignored the effects of collisions in the kinetic region altogether (he used the Langmuir model), which eliminated the need of to solve the Boltzmann equation in this region. The applicability of any of these approximations to the kinetic modelling of Diesel fuel droplet evaporation would require a separate investigation, which has not been performed to the best of our knowledge.

The approach to modelling Diesel fuel droplet evaporation used in [13, 14] is based on the rigorous calculation of the collisional term in the Boltzmann equation using
numerical methods, such as those developed in [21, 13]. The algorithm developed in [13, 14] was specifically designed to model the evaporation and condensation processes in binary mixtures consisting of molecules with different radii and masses. This algorithm was applied to the same problem of evaporation of Diesel fuel into high pressure air as considered earlier in [12], but taking into account the contribution of air molecules. Two regions above the surface of the evaporating droplet were considered. These are the kinetic region, where the analysis was based on the Boltzmann equations for vapour and air, and the hydrodynamic region. Also, it was assumed that the mass fluxes leaving the kinetic region and the corresponding diffusion fluxes in the hydrodynamic region are matched. It was assumed that the vapour mass flux leaving the droplet’s surface is the maximal one (evaporation coefficient is equal to 1). This value of $\beta$ is predicted by the approximate model described in [22] (see Section 2.1 of [14] for a more detailed discussion of this matter). The effects predicted by this model appeared to be noticeable, and larger than those predicted by the approximate analysis, if the contribution of air in the kinetic region was taken into account. It was recommended that the kinetic effects are taken into account when accurate analysis of Diesel fuel droplet evaporation is essential. As shown in our previous paper [23], even relatively small differences in the predicted droplet evaporation time can lead to noticeable differences in the timing of the autoignition in Diesel engine-like conditions.

One of the main limitations of the model described in [13, 14] is that the authors did not take into account the contribution of the heat flux in the kinetic region, assuming that there is no temperature gradient within it. This assumption could not be justified without solving a more general problem, taking into account this effect. This is done in the present paper. The algorithm of the solution of the Boltzmann equation is the same as used in [13, 14], but the effects of the heat flux in the kinetic region are taken into account (this leads to an additional non-trivial problem of formulating the boundary conditions for temperature). Also, an updated version of the hydrodynamic model is used. In contrast to [14], more accurate expressions for the binary diffusion coefficient and the convection heat transfer coefficient are used, and the temperature dependence of the fuel vapour specific heat capacity and thermal conductivity is taken into account.

The physical model is briefly described in Section 2. A new algorithm for calculating the fuel vapour density and temperature at the outer boundary of the kinetic region is described in Section 3. The results of calculations of the evolution of Diesel fuel droplet radii and temperature during the heating and evaporation process, for typical engine parameters, are presented and discussed in Section 4. The main results of the paper are summarised in Section 5.

## 2 Physical model

As in [12, 14], two regions of gas above the surface of the evaporating fuel droplet are considered: the kinetic and hydrodynamic regions. These are schematically shown in Fig. 1. As in [14], we assume that gas consists of two components, fuel vapour and background air, both in the kinetic and hydrodynamic regions. It is assumed that the contribution of chemical reactions of fuel vapour and oxygen can be ignored. Fuel
vapour and air dynamics in the first region are described by the Boltzmann equations, while the conventional hydrodynamic analysis is applied in the second region. This means that we investigate a two surface problem. As in [14], the effects of droplet motion, thermal radiation and the temperature gradient inside droplets are ignored. None of these assumptions can be rigorously justified in Diesel engine-like conditions but they allow us to separate these effects from the kinetic effects. In a comprehensive model these effects will need to be taken into account alongside the kinetic effects.

2.1 Kinetic region

As in [13, 14], the evolution of the molecular velocity distribution functions of air \( f_a \equiv f_a(r, t, v) \) and fuel vapour \( f_v \equiv f_v(r, t, v) \) in the kinetic region is controlled by the corresponding Boltzmann equations:

\[
\begin{align*}
\frac{\partial f_a}{\partial t} + v_a \frac{\partial f_a}{\partial r} &= J_{aa} + J_{av} \\
\frac{\partial f_v}{\partial t} + v_v \frac{\partial f_v}{\partial r} &= J_{va} + J_{vv}
\end{align*}
\]

(2)

where \( J_{\alpha\beta} (\alpha = a, v; \beta = a, v) \) are collision integrals defined as:

\[
J_{\alpha\beta} = \frac{\sigma_{\alpha\beta}^2}{2} \int_{-\infty}^{+\infty} dv_1 \int_0^\pi d\theta d\phi \int_0^{2\pi} d\phi \left( f_\alpha f_\beta^\prime_1 - f_\alpha f_\beta^\prime \right) |v_\alpha - v_\beta|,
\]

(3)

\( \sigma_{\alpha\beta} = (\sigma_\alpha + \sigma_\beta)/2 \), \( \sigma_\alpha \) and \( \sigma_\beta \) are the corresponding diameters of molecules, \( \theta \) and \( \phi \) are angular coordinates of molecules \( \beta \) relative to molecules \( \alpha \) after the collision, superscript \( \prime \) indicates the velocities and the molecular velocity distribution functions after collisions (in what follows these functions will be referred to as ‘molecular distribution functions’). Subscript \( 1 \) indicates that molecules of type \( \beta \) collide with molecules of type \( \alpha \) and as a result of this interaction the function \( f_\alpha \) is modified. The first integral on the right hand side of (3) is calculated in the three dimensional velocity space. When deriving (2) and (3) it was assumed that molecules are rigid elastic spheres and that body forces acting on them are negligible.

The analysis of the system of Equations (2) is the same as in [13, 14] except that both mass and heat transfer in the kinetic region are taken into account. As in [14] it is assumed that the evaporation coefficient \( \beta \) is equal to 1. In contrast to [14], the changes of temperature across the kinetic region are taken into account.

2.2 Hydrodynamic region

As in [14], it is assumed that the mass fluxes leaving the kinetic region and the corresponding diffusion fluxes in the hydrodynamic region are matched. In contrast to [14], however, the difference between the area of the outer surface of the kinetic region and the area of the droplet surface is ignored. The validity of this assumption was checked by a direct comparison of the results, taking and not taking into account the effects of the sphericity of droplets for the thickness of the kinetic region equal to ten mean molecular paths, calculated for the pressure equal to 30 bars (Diesel engine-like conditions) and temperatures equal to fuel droplet surface temperatures (see Section 3.1 and
Equation (11) of [14]). As a result, the mass flux matching condition is presented in the form:

\[
\frac{M_v}{N_A} \int_{-\infty}^{+\infty} dv_x \int_{-\infty}^{+\infty} dv_y \int_{0}^{+\infty} dv_z f_v(r,t,v) = \frac{\rho_{mix} D_{va}}{R_d} \ln (1 + B_M) \equiv j_{hyd} = j_v, \tag{4}
\]

where \(\rho_{mix}\) is the density of the mixture of air and vapour at the inner boundary of the hydrodynamic region (\(\rho_{mix} = \rho_{vRD}/Y_{vRD}\)), \(D_{va}\) is the binary diffusion coefficient (diffusion of vapour through air), \(B_M = Y_{vRD}/(1 - Y_{vRD})\) is the Spalding mass transfer number, \(Y_{vRD}\) is the fuel vapour mass fraction at the inner boundary of the hydrodynamic region, \(j_{hyd}\) is the mass flux of evaporated fuel. \(B_M\) takes into account the effect of the finite mass fraction of fuel vapour on the evaporation process (see Section 3.2.1 of [24] for the details). The binary diffusion coefficient is calculated from the following expression [25]:

\[
D_{va} = 1.8583 \times 10^{-7} \sqrt{T_r^3 \left( \frac{1}{M_v} + \frac{1}{M_a} \right)} \frac{1}{p \sigma_{va}^2 \Omega_{D,va}}, \tag{5}
\]

where \(D_{va}\) is in m\(^2\)/s, \(p\) is in atm (1 atm \(\approx 1.01 \times 10^5\) Pa), \(\sigma_{va} = 0.5(\sigma_v + \sigma_a)\) is the average diameter of molecules of vapour and air (in \(\text{m} \times 10^{-10}\)), \(\Omega_{D,va}\) is the function of \(T^* \equiv k_B T_r/\varepsilon_{va}\), \(\varepsilon_{va} = \sqrt{\varepsilon_v \varepsilon_a}\), \(\varepsilon_v\) and \(\varepsilon_a\) are Lennard-Jones parameters for fuel vapour and air [25], \(k_B\) is the Boltzmann constant, \(T_r = T_s + \frac{1}{3} (T_g - T_s)\) is the reference temperature, \(T_s\) is the droplet surface temperature, \(T_g\) is the ambient gas temperature.

In accordance with [25] the following approximation for \(\Omega_{D,va}\) is used:

\[
\Omega_{D,va} = \frac{1.06036}{T^{0.15610}} + \frac{0.19300}{\exp(0.47635T^*)} + \frac{1.03587}{\exp(1.52996T^*)} + \frac{1.76474}{\exp(3.89411T^*)}.
\]

The following values are used for most of our analysis: \(\sigma_v = 7.463 \times 10^{-10}\) m, \(\sigma_a = 3.617 \times 10^{-10}\) m, \(\varepsilon_v/k_B = 351.0\) K, and \(\varepsilon_a/k_B = 97.0\) K [25]. It was assumed that n-dodecane can be approximated by \(\text{C}_9\text{H}_{22}\) in this case. These values are different from those used in [14], where the analysis was based on [26]. The chosen values of these parameters are between those recommended by [26] and a more recent paper [27].

The heat flux supplied to the droplet is estimated as:

\[
q_s = h(T_g - T_s), \tag{6}
\]

where the convection heat transfer coefficient \(h\) is obtained from the equation [28]-[30]:

\[
h = \frac{k_{mix}}{R_d} \ln (1 + B_T) B_T, \tag{7}
\]

\(k_{mix}\) is the thermal conductivity of the mixture of vapour and air, \(B_T\) is the Spalding heat transfer number calculated as [28]:

\[
B_T = (1 + B_M)^\varphi - 1, \tag{8}
\]

\[
\varphi = \left( \frac{c_{pv}}{c_{pg}} \right) \frac{1}{Le}, \tag{9}
\]
Le = \frac{k_g}{(c_{pv}\rho_{mix}D_{ca})} is the Lewis number, \( c_{pv} \) and \( c_{pg} \) are specific heat capacities of the fuel vapour and ambient gas (air), respectively, \( k_g \) is the ambient gas thermal conductivity.

Note that, strictly speaking, the value of \( T_s \) in Equation (6) should have been replaced by gas temperature in the immediate vicinity of the droplet surface (\( T_{gs} \)). \( T_{gs} \) is slightly higher than \( T_s \) due to the temperature jump predicted by the kinetic theory [31]-[36]. As follows from our analysis for Diesel engine-like conditions, presented later in this paper, the value of \( (T_{gs} - T_s)/T_s \) does not exceed 0.5%. This leads to our overestimate of \( q_s \) and \( \tilde{T}_{Rd} - 1 \equiv (T_{Rd}/T_s) - 1 \) by not more than approximately 0.5% (see Fig. 4b). Also, it follows from our analysis that \( \tilde{T}_{Rd} - 1 \) does not exceed 0.04. Hence, the value of \( T_{Rd} - T_s \) is expected to be overestimated by 0.005 \times 0.04 = 2 \times 10^{-4} \times 0.04 T_o = 2 \times 10^{-4} T_o \), which can be safely ignored in our analysis. This can justify the application of Equation (6) on which this analysis is based.

The evolution of droplet surface temperatures with time is found from the following equation:

\[
\frac{dT_s}{dt} = \frac{3}{R_d \rho_{li} c_l} (q_s - j_v L),
\]

where \( \rho_l \), \( c_l \), and \( L \) are liquid density, liquid specific heat capacity and latent heat of evaporation. When deriving Equation (10), the effects of temperature gradient inside droplets were ignored (see [24, 37, 38, 39] for a discussion of the validity of this approximation).

The following approximations are used, following [40]:

\[
L = 37440 \cdot (T_{cr} - T_s)^{0.38} \quad J/kg,
\]

\[
\rho_l = 744.11 - 0.771 \cdot (T_s - 300) \quad kg/m^3,
\]

\[
c_l = 2180 + 4.1 \cdot (T_s - 300) \quad J/(kg \cdot K),
\]

\[
k_v = 0.02667 \cdot (T_r/300)) - 0.02087 \quad W/(m \cdot K),
\]

where \( T_{cr} = 659 \) K is the n-dodecane critical temperature, \( T_r \) is the reference temperature, defined earlier.

The values of \( c_{pv} \) are estimated as [38]:

\[
c_{pv} = 1594.60 + 1.15\tilde{T} - 100.56\tilde{T}^2 - 28.56\tilde{T}^3 + 5.07\tilde{T}^4 - 0.25\tilde{T}^5 \quad J/(kg \cdot K),
\]

where \( \tilde{T} = (T_r - 300)/300. \)

The values of \( k_a \) are estimated as [41]:

\[
k_a = 3.227 \cdot 10^{-3} + 8.3894 \cdot 10^{-5} \cdot T_r - 1.9858 \cdot 10^{-8} \cdot T_r^2 \quad W/(m \cdot K).
\]

Following [14], the values of the saturated fuel vapour pressure are estimated as:

\[
p_{v (sat)} = A_1 \cdot \exp \left( \frac{T_s - A_0}{B_1} \right) \quad Pa,
\]

\[
(11)
\]
where
\[
\begin{align*}
A_0 &= 449.87125 \\
A_1 &= 46204.48272 \\
B_1 &= 56.97142 \\
A_0 &= 300.17542 \\
A_1 &= 70.44441 \\
B_1 &= 22.36885
\end{align*}
\] when \( T_s < 440 \) K
\[
\begin{align*}
A_0 &= 300.17542 \\
A_1 &= 70.44441 \\
B_1 &= 22.36885
\end{align*}
\] when \( T_s \geq 440 \) K.

Thermal conductivity of the mixture of fuel vapour and air is estimated as [25, 38]
\[
k_{\text{mix}} = \sum_{i=1}^{2} \frac{X_i k_i}{\sum_{j=1}^{2} X_j \Phi_{ij}} \frac{W}{(m \cdot K)},
\]
where \( i \) and \( j \) stand for fuel vapour or air, \( X_{i,j} \) are molar fractions of species \( i \) and \( j \),
\[
\Phi_{ij} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_i}{M_j} \right)^{-1/2} \left[ 1 + \left( \frac{k_i}{k_j} \right)^{1/2} \left( \frac{M_j}{M_i} \right)^{1/4} \right]^2,
\]
\( M_{i,j} \) are molar masses of the corresponding species (\( M_v = 170.3 \) kg/kmol, \( M_a = 28.97 \) kg/kmol [25]). Note that there is a printing mistake in the expression for \( \Phi_{ij} \) given in [42] (see their Equation (10-6.2)). The specific heat capacities and densities of mixtures were calculated based on the mass fractions of the components.

The processes in the kinetic and hydrodynamic regions are linked by the matching conditions of conservation of mass and heat fluxes at the interface:
\[
\begin{align*}
\dot{j}_{\text{kin}} &= \dot{j}_{\text{hyd}}, \quad (12) \\
q_{\text{kin}} &= q_{\text{hyd}}, \quad (13)
\end{align*}
\]
where subscripts \( \text{kin} \) and \( \text{hyd} \) refer to kinetic and hydrodynamic regions respectively.

### 3 Calculation method

One of the difficulties in calculating mass and heat flux in the model described in the previous section lies in the estimate of the thickness of the kinetic region. In our previous paper [14], this problem was bypassed by observing that the mass flux at the outer boundary of the kinetic region is proportional to the difference between the fuel vapour density at the surface of the droplet and the outer boundary of the kinetic region. The values of the vapour density at the outer boundary of the kinetic region, where mass fluxes in the kinetic and hydrodynamic regions coincide, gave the ‘true’ values of vapour density at this boundary and the corresponding values of the vapour mass flux. Unfortunately this approach proved not to be applicable to our problem when both the vapour density and temperature at the outer boundary of the kinetic region (\( \rho_{Rd} \) and \( T_{Rd} \)) are not known. Hence, the problem of calculating the thickness of the kinetic region has to be revisited. This is done in the next subsection, before the new method.
of calculating the values of $\rho_{Rd}$ and $T_{Rd}$ is described. Once these parameters have been found, the Boltzmann equations (2) are solved in the kinetic region, subject to the new boundary conditions at its outer boundary, following the procedure already described in [13, 14].

3.1 Thickness of the kinetic region

Numerous coupled solutions of the Boltzmann and Navier-Stokes hydrodynamic equations for various mixtures are reported in [43, 44]. In these papers, it is shown that in the case where the thickness of the kinetic region is chosen to be about 10 mean free molecular path lengths ($\lambda_c$), good matching of the kinetic and hydrodynamic solutions can be achieved. In this case the combined kinetic/hydrodynamic solution agreed well with the kinetic solution in the whole domain. Note that transient solutions of both Navier-Stokes and Boltzmann equations were obtained. The matching of these solutions was performed at each time step. The solutions of the Boltzmann equations were used as the boundary conditions for the hydrodynamic equations.

To check whether this estimate is applicable for the mixture of n-dodecane and air at temperatures and pressures typical for Diesel engines, two test problems were considered.

In the first problem, a mixture of n-dodecane and air was contained between two parallel plates. The left plate was kept at temperature $T_s = T_0 = 600$ K, while the right plate was kept at temperature $1000$ K. The left plate was the source of outgoing fuel molecules, and it served as a reflector for incoming fuel vapour and air molecules. The right plate was a sink of fuel vapour molecules, but it could be freely penetrated by air molecules. Gas pressure between the plates was maintained equal to 30 bar. This is a realistic pressure in Diesel engine-like conditions [16]. We have not considered higher gas pressures, expected to be used in future generation Diesel engines [16], as in this case the system is expected to approach the supercritical state and new effects would need to be taken into account alongside the real gas effects (the possibility of ignoring real gas effects for the chosen values of parameters was discussed in [14]).

The partial pressure of vapour at the surface of the left plate was maintained at the saturation level $p_0 = p_s(T_0)$, while this vapour pressure at the right plate was assumed to be equal to zero. The distance between the plates was assumed equal to 100 mean free path lengths for n-dodecane $\lambda_c$ at temperature $T_0$ and pressure $p_s(T_0)$. The problem was to find a steady-state distribution of temperature and number density of fuel vapour between the plates.

Two solutions to this problem were obtained. Firstly, the problem was solved based on Equations (2) in the whole domain. Secondly, the problem was solved using hydrodynamic equations in the whole domain except in the regions up to $10\lambda_c$ away from each of the plates. In this case, the solutions near the plates were obtained based on Equations (2) (kinetic solution). The hydrodynamic and kinetic solutions were matched at distances $10\lambda_c$ from each plate following the procedure described in Section 2. The results of calculations are shown in Fig. 2 in the form of the plots of $\tilde{T}_v \equiv T_v/T_0$ and $\tilde{n}_v = n_v/n_{v0}$ versus $\tilde{x} = x/\lambda_c$, where $n_v$ is the vapour number density (the number of molecules per unit volume), $n_{v0}$ is the vapour number density corresponding to $p_s(T_0)$,
$x$ is the distance from the left plate. Plots (1) in this figure correspond to the case of the solution of the Boltzmann equation in the whole domain, while plots (2) refer to the combined kinetic/hydrodynamic solution. As one can see from this figure, both sets of plots are very close, and this justifies the application of the combined kinetic/hydrodynamic model with the thickness of the boundary layer equal to $10\lambda_c$. In the case where this thickness was taken equal to $5\lambda_c$, the combined kinetic/hydrodynamic solution could not be obtained. We could not identify the exact reason for this, but it seems that this is related to the underlying physics of the model for this thickness of the kinetic region rather than to the properties of the numerical scheme.

In the second problem, a one-dimensional evaporation of liquid n-dodecane into air was considered, assuming that the total pressure is equal to 30 bar and the liquid surface temperature is equal to 600 K. As in the previous problem, two regions above the surface were considered as shown in Fig. 1, with the values of the thickness of the kinetic region equal to $10\lambda_c$ and $50\lambda_c$. The corresponding plots of $\tilde{n}_v = n_v/n_{v0}$ versus $\tilde{x} = x/\lambda_c$ are shown in Fig. 3. As follows from this figure, the values of $n_v$ predicted for both thicknesses of the kinetic region are almost indistinguishable. This justifies our assumption that the thickness of the kinetic region is equal to $10\lambda_c$.

Note that our estimate of $\lambda_c$ did not take into account the surface effects, which can be justified for small Kn (see [45] for the details).

### 3.2 Fuel vapour density and temperature at the boundaries

Once the minimal thickness of the kinetic region have been estimated to be equal to $\delta_{Rd} = 10\lambda_c$, the next task is to find the values of fuel vapour density and temperature at its boundaries. The temperature at the surface of the droplet ($T_s$) is found from Equation (10). The fuel vapour density at the droplet surface ($\rho_s$) is found from the corresponding partial vapour pressure given by Equation (11), assuming that the ideal gas law is valid. However, finding the values of these parameters at the outer boundary of the kinetic region is not trivial. In [14] it was assumed that $T_{Rd} = T_s$. This, however, could not be a priori justified, and this assumption led to physical inconsistency of the formulation of the problem. It led to the conclusion that there is no heat flux in the kinetic region. In this paper, this assumption is relaxed, so that both $\rho_{Rd}$ and $T_{Rd}$ need to be found. These parameters cannot be arbitrarily chosen. They depend on the processes on the droplet surface, and on the mass and heat transfer processes in the hydrodynamic region. Ultimately these values need to be found from the matching conditions (12) and (13).

The first step in the solution of these equations is to perform an investigation of mass and heat transfer processes in the kinetic region for a set of values of $\rho_{Rd}$ and $T_{Rd}$. Remembering the physical background of the problem under consideration (heating and evaporation of droplets in a hot gas), these parameters are considered in the ranges: $\rho_{Rd} < \rho_s$ and $T_{Rd} > T_s$. During the droplet heating process the temperature decreases away from the droplet; the evaporation process is possible when the fuel vapour density decreases away from the droplet surface. Once the values of $\rho_{Rd}$ and $T_{Rd}$ have been found, the solution of the Boltzmann equations (2) in the kinetic region allows us to calculate the mass and heat fluxes at the outer boundary of this region. The calculations
are performed for the normalised values of these fluxes:

\[ \tilde{j}_{\text{kin}} = j_{\text{kin}} / (\rho_0 \sqrt{R_v T_0}), \quad \tilde{q}_{\text{kin}} = q_{\text{kin}} / (p_0 \sqrt{R_v T_0}), \]

where \( R_v \) is the gas constant referring to fuel vapour, \( T_0 \) is the reference temperature arbitrarily chosen as equal to 600 K, \( p_0 \) is the saturated fuel vapour density corresponding to \( T_0 \), fuel vapour density \( \rho_0 \) is calculated from the ideal gas law.

Firstly, it was assumed that \( \rho_{Rd} = 0.95 \rho_s \) and \( T_s = T_0 \). The values of \( \tilde{q}_{\text{kin}} \) were calculated for a wide range of \( \tilde{T}_{Rd} = T_{Rd}/T_0 \) from 1 to 1.5. The results are shown in Figs. 4a,b. As follows from this figure, the dependence of \( \tilde{q}_{\text{kin}} \) on \( \tilde{T}_{Rd} \) is well described by a linear function in the whole range of \( \tilde{T}_{Rd} \) under consideration. The same conclusion was obtained for other values of \( T_s \) in the range 300 K (room temperature) to 659 K (critical temperature).

At the next stage, the effect of \( \rho_{Rd} \) on the values of \( \tilde{q}_{\text{kin}} \) was investigated. The plots of \( \tilde{q}_{\text{kin}} \) versus \( \tilde{\rho}_{Rd} = \rho_{Rd}/\rho_0 \) for four \( \tilde{T}_{Rd} \) are shown in Fig. 5. As follows from this figure, the dependence of \( \tilde{q}_{\text{kin}} \) on \( \tilde{\rho}_{Rd} \) is weak for all temperatures. For \( \tilde{T}_{Rd} \leq 1.1 \) (the most important range for practical applications) this dependence can be ignored altogether. This result is very important for our analysis as it allows us to decouple the effects of \( \tilde{T}_{Rd} \) and \( \tilde{\rho}_{Rd} \) on \( \tilde{q}_{\text{kin}} \).

At the next stage, the dependence of \( \tilde{j}_{\text{kin}} \) on \( \tilde{\rho}_{Rd} \) was investigated, assuming that \( \tilde{T}_{Rd} = 1.05 \) and \( T_s = T_0 \). The results are shown in Fig. 6 for \( \tilde{\rho}_{Rd} \) in the range 0.5 to 0.8. As follows from this figure, \( \tilde{j}_{\text{kin}} \) decreases linearly with increasing \( \tilde{\rho}_{Rd} \). Essentially the same linear dependence of \( \tilde{j}_{\text{kin}} \) on \( \tilde{\rho}_{Rd} \) was found for other values of \( \tilde{T}_{Rd} \) in the range 1 to 1.5 and \( T_s \) in the range 300 K to 659 K.

Having established the above properties of \( \tilde{q}_{\text{kin}} \) and \( \tilde{j}_{\text{kin}} \), the following algorithm for the calculation of \( \rho_{Rd} \) and \( T_{Rd} \) is suggested:

1. Calculate the value of \( q_{\text{hyd}} \) using Equation (6);
2. Take a realistic value of \( \tilde{\rho}_{Rd} \) (0.95 for a Diesel engine-like environment) and draw the plot of \( \tilde{q}_{\text{kin}} \) versus \( \tilde{T}_{Rd} \) as shown in Fig. 4 (as mentioned earlier, the results are expected to remain the same, if a different but reasonable value of this parameter has been chosen; cf. Fig. 5);
3. Find the intersection of the line \( \tilde{q}_{\text{hyd}} = q_{\text{hyd}} / (p_0 \sqrt{R_v T_0}) \) with this plot as shown in Fig. 4b. This intersection gives the required values of \( \tilde{T}_{Rd} \) and \( T_{Rd} \);
4. For the value of \( T_{Rd} \) found in the previous step, calculate the value of \( j_{\text{hyd}} \) from Equation (4);
5. Draw the plot of \( \tilde{j}_{\text{kin}} \) versus \( \tilde{\rho}_{Rd} \) as shown in Fig. 6;
6. Find the intersection of the line \( \tilde{j}_{\text{hyd}} = j_{\text{hyd}} / (\rho_0 \sqrt{R_v T_0}) \) with this plot as shown in Fig. 6. This intersection gives the required values of \( \tilde{\rho}_{Rd} \) and \( \rho_{Rd} \).

4 Results

The algorithm described in the previous section is applied to computation of the heating and evaporation of Diesel fuel droplets of various radii in a hot gas at various temperatures. The initial droplet temperature in all cases is assumed equal to 300 K, and gas pressure is assumed equal to 30 bar. Three approximations were used for calculations.
Firstly, both heat and mass transfer in the kinetic region were taken into account, as described in Section 3. Secondly, mass transfer in the kinetic region was taken into account but not heat transfer (it was assumed that \( T_{Rd} = T_s \)). Thirdly, no kinetic effects were taken into account and the whole problem was solved according to hydrodynamic approximation.

The results of calculation of the heating and evaporation of droplets with initial radius \( R_{d0} = 5 \, \mu m \) immersed into gas with temperature 750 K are shown in Fig. 7. As follows from this figure, kinetic effects lead to visible increase in droplet evaporation time and increase in their temperature, in agreement with the results of our previous studies [12]-[14]. The difference between results predicted by the models taking and not taking into account the effects of heat flux in the kinetic region is negligible. The evaporation times predicted by the hydrodynamic model, the kinetic models ignoring the heat flux in the kinetic region, and taking this flux into account, are 1.254 ms, 1.285 ms and 1.291 ms respectively; the values of the normalised temperatures at these times are predicted to be 0.883, 0.896 and 0.898 respectively. Essentially the same conclusions follow from the observation of Fig. 8, where the same results as in Fig. 7, but for \( R_{d0} = 20 \, \mu m \), are presented. Comparing Figs. 6 and 7 one can see that the increase in droplet radii leads to a decrease in the kinetic effects (droplet radii and temperatures predicted by kinetic and hydrodynamic models become closer). Note that the difference between the plots shown in Fig. 7 and the corresponding plots shown in Fig. 14 of [14] can be mainly attributed to the different models for the convection heat transfer coefficient (see Equation (7)) and the different values of the parameters of n-dodecane molecules (these control the value of the binary diffusion coefficient; see Equation (5)) used. The same remark refers to Fig. 9 of this paper and Fig. 16 of [14].

The same plots as in Figs. 7 and 8 but for gas temperature 1000 K are shown in Figs. 9 and 10. As can be seen from these figures, in the case of the hotter gas, the effects of heat transfer in the kinetic region become clearly visible. For droplets with \( R_{d0} = 5 \, \mu m \) the predicted evaporation time in the presence of heat flux in the kinetic region turned out to be about 4.8% longer than predicted by the hydrodynamic model. The increase in this time in the case where the heat flux in the kinetic region is ignored would only be about 2.8%.

The same plots as in Figs. 7-10 but for gas temperature 1500 K are shown in Figs. 11 and 12. As can be seen from these figures, in the case of this gas temperature, the effects of heat transfer in the kinetic region become even more important than in the previous cases. For droplets with \( R_{d0} = 5 \, \mu m \) the predicted evaporation time in the presence of heat flux in the kinetic region proved to be about 14% longer than predicted by the hydrodynamic model. The increase in this time in the case where the heat flux in the kinetic region is ignored would only be about 8%.

The slowing down of the evaporation processes due to the presence of the heat flux in the kinetic region is related to the increased gas temperature near the outer boundary of the kinetic region. The fuel vapour molecules leaving the surface of the droplets are more likely to return to this surface when they encounter this region of increased temperature. The evaporation process itself is not affected by the droplet radii. However, the relative contribution of the evaporation process is expected to be more visible for the small droplets than for the large ones, which is confirmed by our
Finally, the sensitivity of the results to the choice of the diameter on n-dodecane molecules was investigated. The results shown in Fig. 7 for the hydrodynamic model and the kinetic model, taking into account the effects of heat transfer in the kinetic region, were compared with similar results obtained for \( \sigma_n = 9.373 \times 10^{-10} \text{m} \). This value for the diameter of n-dodecane molecules was given in [26]. The relevant plots are shown in Fig. 13. As follows from this figure, for both molecular diameters the kinetic effects have almost identical impact on the values of droplet radii and temperature, although the droplet evaporation time is visibly shorter for smaller molecules. Similar conclusions were obtained for the initial droplet radius 20 \( \mu \text{m} \) and gas temperatures 1000 and 1500 for both droplet radii.

5 Conclusions

The previously developed kinetic model for droplet heating and evaporation into a high pressure background gas (air) has been generalised to take into account the contribution of heat flux in the kinetic region in the vicinity of the droplet surface. The dynamics of molecules in this region are described in terms of the Boltzmann equations for vapour and air. The boundary conditions at the outer boundary of the kinetic region are introduced by matching the mass fluxes of vapour leaving the kinetic region and entering into the surrounding hydrodynamic region, and the corresponding heat fluxes. The thickness of the kinetic region is estimated to be equal to about 10 mean free molecular path lengths, estimated at the temperature equal to the droplet surface temperature.

It is pointed out that for the parameters typical for Diesel engine-like conditions, heat flux in the kinetic region is a linear function of the vapour temperature at the outer boundary of the kinetic region, but practically does not depend on vapour density at this boundary. On the other hand, the mass flux at this boundary decreases almost linearly with increasing vapour density at the same location. Remembering these properties of the heat and mass fluxes, and using the matching conditions at the outer boundary of the kinetic region, the values of temperature and fuel vapour density at this boundary are found.

The model is applied to the simulation of heating and evaporation of fuel droplets in Diesel engine-like conditions. It is pointed out that in the case of droplet heating in a relatively cool gas \( T_g = 750 \text{ K} \) the effect of non-zero heat flux in the kinetic region is negligible. This effect, however, turns out to be important in the cases where gas temperature rises to 1000 K and 1500 K. For the latter temperature, for droplets with initial radii \( R_{d0} = 5 \mu \text{m} \), the predicted evaporation time in the presence of heat flux in the kinetic region is about 14% longer than predicted by the hydrodynamic model. The increase in this time in the case where the heat flux in the kinetic region is ignored is only about 8%. In agreement with the previously reported results, the importance of kinetic effects increases with decreasing droplet radii. The application of the rigorous kinetic model, taking into account the heat flux in the kinetic region, as described in this paper, is recommended when accurate predictions of the values of droplet surface temperature, evaporation time and autoignition delay in Diesel engine-like conditions.
are essential.

**Nomenclature**

$A_{0,1}, B_1$ coefficients introduced in Equation (11)
$B_M$ Spalding mass transfer number
$B_T$ Spalding heat transfer number
$c$ specific heat capacity
$D$ binary diffusion coefficient
$f$ molecular velocity distribution function
$h$ convection heat transfer coefficient
$j$ mass flux
$J$ collision integral
$k$ thermal conductivity
$k_B$ Boltzmann constant
$Kn$ Knudsen number
$L$ specific heat of evaporation
$Le$ Lewis number
$M$ molar mass
$n$ number density
$N_A$ Avogadro number
$q$ heat flux
$p$ pressure
$r$ radius-vector
$R_v$ gas constant referring to fuel vapour
$R_d$ droplet radius
$\tilde{R}$ $R_d/R_{d0}$
$t$ time
$T$ temperature
$\tilde{T}_v$ $T_v/T_0$
$\tilde{T}$ $(T_s - T_{s0})/(T_{cr} - T_{s0})$
$\tilde{T}_{Rd}$ $T_{Rd}/T_0$
$T^* = k_B T_r/\varepsilon_{va}$
$v$ velocity (components)
$v$ velocity (vector)
$X$ molar fraction
$Y$ mass fraction

**Greek symbols**

$\beta$ evaporation coefficient
$\delta_{Rd}$ thickness of the kinetic region
$\varepsilon_{va} = \sqrt{\varepsilon_v \varepsilon_a}$
$\varepsilon_v, \varepsilon_a$ Lennard-Jones parameters for fuel vapour and air
$\theta$ angular coordinate
$\lambda_c$ mean free molecular path length
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>density</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>diameter of molecules</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>parameter defined by Equation (8)</td>
</tr>
<tr>
<td>$\phi$</td>
<td>angular coordinate</td>
</tr>
<tr>
<td>$\Omega_{D,v}^{a}$</td>
<td>parameter introduced in Formula (5)</td>
</tr>
</tbody>
</table>

**Subscripts**
- $a$ : air
- $\alpha, \beta$ : $\alpha = a, v$; $\beta = a, v$
- cr : critical
- $d$ : droplet
- hyd : hydrodynamic
- kin : kinetic
- $g$ : gas
- $l$ : liquid
- mix : mixture
- $r$ : reference
- $Rd$ : outer boundary of the kinetic region
- $s$ : surface
- sat : saturated
- $v$ : fuel vapour
- $0$ : initial or reference

**Superscripts**
- $'$ : after the collision
- $\sim$ : normalised

---

**Acknowledgments**

The authors are grateful to A.P. Kryukov, V.Yu. Levashov and M.R. Heikal for their support and useful discussions. The Royal Society, EPSRC (Grant EP/E02243X/1) (UK) and Russian fund for fundamental research (Grant 08-08-12195) are acknowledged for the financial support of this project.

**References**


Figure Captions

Fig. 1 Kinetic and hydrodynamic regions above the surface of the droplet. $T_s$ is the droplet surface temperature, $\rho_s$ is the fuel vapour density in the immediate vicinity of the droplet surface, $T_{Rd}$ and $\rho_{Rd}$ are the temperature and density of vapour at the outer boundary of the kinetic region. $\delta_{Rd}$ indicates the thickness of the kinetic region, $j_v$ and $q$ show the directions of the vapour mass and heat fluxes respectively.

Fig. 2 Plots of $\tilde{T}_v \equiv T_v/T_0$ and $\tilde{n}_v = n_v/n_{v0}$ versus $\tilde{x} = x/\lambda_c$, where $n_v$ is the vapour number density, $n_{v0}$ is the vapour number density corresponding to $p_s(T_0)$, $x$ is the distance from the left plate. Plots (1) correspond to the case of the solution of the Boltzmann equation in the whole domain, while Plots (2) refer to the combined kinetic/hydrodynamic solution.

Fig. 3 Plots of $\tilde{n}_v = n_v/n_{v0}$ versus $\tilde{x} = x/\lambda_c$, describing the evaporation of liquid n-dodecane into ambient air, where $n_v$ is the vapour number density, $n_{v0}$ is the vapour number density corresponding to $p_s(T_0)$, $x$ is the distance from the liquid surface. Plots (1) and (2) correspond to the cases of the thickness of the kinetic region equal to 10$\lambda_c$ and 50$\lambda_c$ respectively. The total pressure of the mixture of fuel vapour and air is equal to 30 bar and the liquid surface temperature is equal to 600 K.

Fig. 4 Plots of normalised heat flux in the kinetic region $\tilde{q}_{kin} = q_{kin}/(p_0\sqrt{R_v}T_0)$ versus normalised temperature $\tilde{T}_{Rd} = T_{Rd}/T_0$, assuming that $T_0 = T_s = 600$ K. Figure b shows the magnified section of figure a referring to $0 \leq \tilde{T}_{Rd} \leq 1.1$. It illustrates how the value of $\tilde{T}_{Rd}$ is found based on the previously calculated value of $\tilde{q}_{hyd}$.

Fig. 5 Plots of normalised heat flux in the kinetic region $\tilde{q}_{kin} = q_{kin}/(p_0\sqrt{R_v}T_0)$ versus normalised fuel vapour density $\tilde{\rho}_{Rd} = \rho_{Rd}/\rho_0$ for four values of $\tilde{T}_{Rd}$, indicated near the plots.

Fig. 6 Plots of normalised vapour mass flux in the kinetic region $\tilde{j}_{kin} = j_{kin}/(p_0\sqrt{R_v}T_0)$ versus normalised density $\tilde{\rho}_{Rd} = \rho_{Rd}/\rho_0$, assuming that $\tilde{T}_{Rd} = 1.05$. This plot illustrates the way in which the value of $\tilde{\rho}_{Rd}$ is found, based on the previously calculated value of $\tilde{j}_{hyd}$.

Fig. 7 Plots of $\tilde{R} = R_{d}/R_{d0}$ and $\tilde{T} = (T_s - T_{a0})/(T_{c1} - T_{a0})$ versus time for a Diesel fuel droplet, predicted by the rigorous kinetic model, taking into account the contribution of heat flux in the kinetic region (1), the kinetic model ignoring the contribution of this heat flux (2), and the hydrodynamic model (3). The total pressure is 30 bar, the
initial droplet temperature is 300 K, $R_{d0} = 5 \mu\text{m}$, and $T_g = 750 \text{ K}$. The contribution of air in the kinetic region is taken into account in all cases.

**Fig. 8** The same as Fig. 7 but for $R_{d0} = 20 \mu\text{m}$.

**Fig. 9** The same as Fig. 7 but for $T_g = 1000 \text{ K}$.

**Fig. 10** The same as Fig. 8 but for $T_g = 1000 \text{ K}$.

**Fig. 11** The same as Fig. 7 but for $T_g = 1500 \text{ K}$.

**Fig. 12** The same as Fig. 8 but for $T_g = 1500 \text{ K}$.

**Fig. 13** Plots of $\tilde{R} = R_d/R_{d0}$ and $\tilde{T} = (T_s - T_{s0})/(T_{cr} - T_{s0})$ versus time for a Diesel fuel droplet, predicted by the rigorous kinetic model, taking into account the contribution of heat flux in the kinetic region (Plots (1) and (3)), and by the hydrodynamic model (Plots (2) and (4)). Plots (1) and (2) refer to the case when the diameter of vapour molecules was taken equal to $\sigma_v = 7.463 \times 10^{-10}\text{m}$, following [25]. Plots (3) and (4) refer to the case when the diameter of vapour molecules was taken equal to $\sigma_v = 9.373 \times 10^{-10}\text{m}$, following [26]. The total pressure is 30 bar, the initial droplet temperature is 300 K, $R_{d0} = 5 \mu\text{m}$, and $T_g = 750 \text{ K}$. The contribution of air in the kinetic region is taken into account in all cases.
Fig. 1.
Fig. 2.
Fig. 3.
Fig. 4.
Fig. 5.
Fig. 6.
Fig. 7.
Fig. 8.
Fig. 9.
Fig. 10.
Fig. 11.
Fig. 12.
Fig. 13.