

Available online at www.sciencedirect.com



International Journal of HEAT and MASS TRANSFER

International Journal of Heat and Mass Transfer 47 (2004) 2541-2549

www.elsevier.com/locate/ijhmt

Evaporation of diesel fuel droplets: kinetic versus hydrodynamic models

A.P. Kryukov^a, V.Yu. Levashov^a, S.S. Sazhin^{b,*}

^a Centre of High Technologies, Moscow Power Engineering Institute, Krasnokazarmennaya 14, Moscow 111250, Russia

^b School of Engineering, Faculty of Science and Engineering, University of Brighton, Lewes Road, Cockcroft Building,

Brighton BN2 4GJ, UK

Received 13 November 2003; received in revised form 9 January 2004

Abstract

A comparative analysis of hydrodynamic and kinetic approaches to the problem of diesel fuel droplet evaporation is presented. It is pointed out that the kinetic effects on droplet evaporation are always noticeable, despite the fact that this evaporation takes place at high pressures (up to 30 atm and even more). This shows the limitation of applying the hydrodynamic approach to modelling this process. The hydrodynamic approach is universally used in computational fluid dynamics (CFD) codes. Kinetic models predict longer evaporation time and higher droplet temperature compared with the hydrodynamic model. The kinetic effects are shown to be more pronounced for smaller droplets (5 μ m) than for larger ones (20 μ m). The droplet evaporation time and droplet temperature increase with decreasing evaporation coefficient. It is recommended that kinetic effects are taken into account when modelling the evaporation process of diesel fuel droplets in realistic internal combustion engines.

© 2004 Elsevier Ltd. All rights reserved.

Keywords: Droplet evaporation; Kinetic model; Hydrodynamic model; Diesel fuel

1. Introduction

The importance of accurately modelling diesel fuel droplet evaporation in engineering applications is well known [1–8]. A conventional approach to this modelling is based on the assumption that diesel fuel vapour in the vicinity of the droplet surface is always saturated. The rate of evaporation is essentially controlled by fuel vapour diffusion from the vicinity of the droplet surface to the ambient gas [2,5]. This 'hydrodynamic' approach is universally used in engineering models of diesel fuel droplet evaporation and is incorporated in relevant computational fluid dynamics (CFD) codes (e.g. [9–12]). It implicitly assumes that the rate of detachment of molecules of diesel fuel is such that the concentration of fuel vapour at the droplet surface is maintained at the saturation level. The applicability of this assumption to the problem of modelling of diesel fuel droplet evaporation in realistic diesel engines is not at first evident. In order to check it, a more general kinetic model needs to be developed and applied to the solution of this problem.

The main objective of this paper is to perform the modelling of diesel fuel droplet evaporation using hydrodynamic and kinetic approaches and to compare the results. Although the analysis is focused specifically on the problem of diesel fuel droplet evaporation, it can be easily adjusted to describe the evaporation of other liquid droplets. The background of the problem with the emphasis on the previously suggested kinetic models is presented in Section 2. In Section 3 the basic equations used in the analysis are presented. Results of calculations are presented and discussed in Section 4. The main conclusions of the paper are summarised in Section 5.

^{*}Corresponding author. Tel.: +44-127-360-0900; fax: +44-127-364-2301.

E-mail address: s.sazhin@brighton.ac.uk (S.S. Sazhin).

^{0017-9310/\$ -} see front matter 0 2004 Elsevier Ltd. All rights reserved. doi:10.1016/j.ijheatmasstransfer.2004.01.004

Nomenc	lature
--------	--------

$a_{ m f}\ b_{ m f}\ B_{ m M}$	coefficient in Eq. (8) coefficient in Eq. (8) Spalding mass number	R _g T Y	gas constant temperature mass fraction
c d D _c h	specific heat capacity diameter of molecules binary diffusion coefficient convection heat transfer coefficient	Greek s β _m ρ	<i>symbols</i> evaporation (condensation) coefficient density
j _{lg}	mass flux of fuel vapour from the droplet surface	Subscrij a	<i>pts</i> air decelet
к Кп l	Knudsen number molecular mean free path	d dr e	drift evaporation
L Le	specific latent heat of evaporation Lewis number	f K	fuel vapour Knudsen layer
$M \over \dot{m}_{ m d}$	molar mass rate of droplet mass loss	l mix	liquid fuel mixture of fuel vapour and air
N_A N_ρ	Avogadro number $(\rho_{\rm s} - \rho_{\rm Rd})/\rho_{\rm s}$ (T - T)/T	p Rd	constant pressure outer boundary of the Knudsen layer
$p \\ Q$	$(I_{\rm s} - I_{\rm Rd})/I_{\rm s}$ pressure heat rate	sound ∞	sound sound away from droplet surface (outside Knudsen
R _d	droplet radius		layer)

2. Background

The simplest kinetic model for droplet evaporation (condensation) was developed for a free molecular flow near the droplet surface (Knudsen number (*Kn*) is much greater than 1). Assuming that both incoming and outgoing molecular fluxes are Maxwellian with temperatures T_{∞} and $T_{\rm s}$ respectively, one can derive the Hertz–Knudsen–Langmuir formula for mass flux of fuel vapour from the droplet surface [13–18]:

$$j_{\rm lg} = \frac{\dot{m}_{\rm d}}{4\pi R_{\rm d}^2} = \frac{\beta_{\rm m}}{\sqrt{2\pi R_{\rm g}}} \left(\frac{p_{\rm s}}{\sqrt{T_{\rm s}}} - \frac{p_{\infty}}{\sqrt{T_{\infty}}}\right),\tag{1}$$

where $\dot{m}_{\rm d}$ is the rate of droplet mass loss, $R_{\rm d}$ is the droplet radius, $\beta_{\rm m}$ is the evaporation or condensation coefficient, $R_{\rm g}$ is gas constant, $p_{\rm s}$ is the saturated fuel vapour partial pressure corresponding to $T_{\rm s}$, p_{∞} is the fuel vapour partial pressure at large distances from it, $T_{\rm s}$ is the droplet surface temperature and T_{∞} is the gas temperature at large distances from the droplet.

The coefficient $\beta_{\rm m} \leq 1$ shows what portion of vapour molecules striking the liquid surface is absorbed by this surface. The remaining portion $(1 - \beta_{\rm m})$ shows the fraction of reflected molecules. The value of $\beta_{\rm m}$ depends on contacting surfaces [19] and can be determined experimentally [19,20]. Also, methods of molecular dynamics and direct modelling of droplet evaporation could be used to estimate this coefficient [21–23]. Unfortunately, the values of β_m for diesel fuel have not been measured or estimated to the best of our knowledge.

Eq. (1) has been widely used for the analysis of evaporation and condensation processes despite the simplistic assumptions used for its derivation (e.g. [24]). A more general approach to the evaporation–condensation problem takes into account the effects of collisions. This leads to the introduction of the concept of the Knudsen layer, separating the liquid surface from the bulk of the vapour which is described using the continuum equations. The thickness of the Knudsen layer $l_{\rm K}$ is typically estimated as several molecular mean free pass lengths l for small drift vapour velocities $v_{\rm dr}$, 10*l* for $v_{\rm dr} = 0.5v_{\rm sound}$, and 100–200*l* for $v_{\rm dr}$ close to $v_{\rm sound}$ [25]. The value of l is estimated based on the temperature equal to $T_{\rm s}$.

Diesel fuel droplets can be approximated by ndodecane $C_{12}H_{26}$ ($M_{C_{12}H_{26}} = 170.3$ kg/kmol) for which the gas constant is estimated as $R_g = 48.88$ J/(kg K). Assuming that $T_s = 600$ K we obtain $v_{sound} = 202.6$ m/s. For this T_s the saturated vapour pressure of n-dodecane is equal to $p_s = 6.4 \times 10^5$ N/m². Using Eq. (1), assuming that $p_{\infty} = 0$ and $\beta_m = 0.5$ we obtain $j_{1g} = 745$ kg/(m² s). From gas law we have $\rho_s = 21.8$ kg/m³. Hence, $v_{dr} = j_{1g}/\rho_s = 34$ m/s. This value could be further modified if different β_m are used. In all cases, however, we can assume that $l_{\rm K} < 5l$. Note that this result is not very sensitive to the value of $T_{\rm s}$. For example for $T_{\rm s} = 400$ K we obtain: $v_{\rm sound} = 165$ m/s and $v_{\rm dr} = 28$ m/s. More accurate analysis of the problem (see Eq. (3)) would predict a bit larger values of $v_{\rm dr}$, but the validity of the assumption that $v_{\rm dr} \ll v_{\rm sound}$ would remain valid. Assuming that liquid fuel evaporates into its own vapour, l can be estimated as [16]:

$$l = [\sqrt{2}\pi d_{\rm f}^2(\rho_{\rm s}N_{\rm A})/M_{\rm f}]^{-1}$$

where $M_{\rm f}$ and $d_{\rm f}$ are molar mass and diameter of molecules of the diesel fuel, $N_{\rm A}$ is the Avogadro number.

Taking the diameter of n-dodecane molecules $d = 10^{-9}$ m, $\rho_s = 21.8$ kg/m³ (corresponding to $T_s = 600$ K) and $M_f = 170.3$ kg/kmol, we obtain: $l = 2.9 \times 10^{-9}$ m. This gives us the estimate of l_K for diesel engines: $l_K < 1.5 \times 10^{-8}$ m = 0.015 µm. This is about 2 orders of magnitude less than the droplet radii. As will be shown later in this paper, however, despite the small thickness the contribution of the Knudsen layer cannot be a priori ignored even in dense gases including those in diesel engines. The thickness of the Knudsen layer for the case of fuel evaporation into its own vapour is expected to increase by 1–2 orders of magnitude for $T_s = 400$ K. The rate of evaporation at this temperature, however, is expected to be small.

Note that strictly speaking the Boltzmann equation can be applied only when l is much greater than d [26]. From this point of view the results of our analysis are expected to be reliable only for the set of parameters when the condition $l \gg d$ is satisfied. In the case when lis close to d (which is expected near the critical state) our model can show the trends of the processes, rather than give reliable quantitative estimates. Also, the solutions of the Boltzmann equation, on which our analysis is based, do not take into account the contribution of the processes inside the fuel vapour molecules.

The abovementioned estimates of l and l_K do not take into account the contribution of molecules of air in the Knudsen layer. This can be justified by the small thickness of this layer at temperatures well above room temperature (when the evaporation rate is high enough). The general kinetic theory of liquid fuel evaporation taking into account the contribution of molecules of air in the Knudsen layer has not been developed to the best of our knowledge. Hence the assumption that the liquid fuel evaporates into its own vapour will be held in the rest of the paper.

The velocity distribution for the molecules in the Knudsen layer is affected by collisions and can be obtained from the solution of the Boltzmann equation. Schrage [15] drew attention to the fact that the effects of collisions lead to the formation of the shifted Maxwellian distribution of molecules near the outer boundary of the Knudsen layer. The authors of [27] assumed that this distribution function is formed in the whole Knudsen layer up to the liquid surface. Considering the case when vapour drift velocity is much less than the velocity of sound (weak evaporation; this assumption is consistent with abovementioned estimates)), and using matching boundary conditions in this layer, they derived the modified expression for j_{lg} at $Kn \ll 1$ and $(T_{\infty} - T_s)/T_s \ll 1$. This expression took into account the convection of vapour and collision processes and could be presented in the form:

$$j_{\rm lg} = \frac{2\beta_{\rm m}}{(2-\beta_{\rm m})\sqrt{2\pi R_{\rm g}}} \left(\frac{p_{\rm s}}{\sqrt{T_{\rm s}}} - \frac{p_{\infty}}{\sqrt{T_{\infty}}}\right).$$
(2)

For $\beta_{\rm m} = 1$ this equation predicts the value of $j_{\rm lg}$ twice as much as the one predicted by Eq. (1).

Further development of the kinetic theory of evaporation and condensation was reported in [28-31]. Perhaps the most detailed solution of the one-dimensional evaporation and condensation problem in a semi-infinite space was reported in [31]. The solution was obtained using the moment method and was based on the assumption of discontinuous shifted Maxwellian velocity distributions of molecules inside the Knudsen layer. In this method the rigorous solution of the Boltzmann equation was replaced by the solution of six equations for six moments of velocity distributions: molecular concentration, temperature and normal velocities for incoming and outgoing flows. Macroscopic parameters were calculated as integrals of the velocity distribution function over the three-dimensional velocity space (moments). The results were similar to those which follow from more complicated approximations [31]. The problem was solved using two forms of the collisional term in the Boltzmann equation: the conventional one and the one suggested by Bhatnagar et al. [32]. The latter form of the collisional term secures the conservation of particles during the collision process, and has been widely used to model collisions in gases and plasma (see e.g. [33]). The results turned out to be practically independent on the form of the collision term used.

The analysis performed in [31] allowed the authors to obtain a number of equations useful for computation of dynamics of evaporation and condensation processes, including the one describing the mass flux of vapour leaving the droplet into a dense medium ($Kn \ll 1$):

$$j_{\rm lg} = \frac{\beta_{\rm m}(p_{\rm sat}(T_{\rm s}) - p_{\rm Rd})}{(1 - 0.4\beta_{\rm m})\sqrt{2\pi R_{\rm g} T_{\rm s}}},\tag{3}$$

where $p_{sat}(T_s)$ is the equilibrium pressure of the saturated vapour at surface temperature T_s , p_{Rd} is the vapour pressure just outside the Knudsen layer. Eq. (3) has been widely used in various applications (e.g. [34]). It is valid in the case of weak evaporation and condensation which is expected to take place when $(T_{Rd} - T_s)/T_s \ll 1$. Further development of the theory of weak evaporation has been reported in [35–43]. These developments, however, do not undermine the usefulness of Eq. (3) for practical applications. This equation is more accurate than Eqs. (1) and (2) and will be used in our analysis.

The increase in intensity of evaporation leads to further deformation of the molecular distribution function in the Knudsen layer. At a certain stage, the linearisation of this distribution function (which was used when deriving Eq. (3)) becomes no longer possible. This leads to the situation when v_{dr} becomes comparable with the velocity of sound and the theory of weak evaporation and condensation is no longer valid. Theory of intensive evaporation has been developed in [44–64]. A review of computational and experimental results referring to intensive condensation, with particular emphasis on the problem of the determination of β_m , was presented in [65].

Results of calculations allowed the authors of [50] to approximate the mass flux of vapour leaving the droplet by the following expression (valid for both weak and strong evaporation):

$$j_{\rm lg} = 0.6\sqrt{2R_{\rm g}T_{\rm s}}(\rho_{\rm s}-\rho_{\rm Rd})\sqrt{\rho_{\rm Rd}/\rho_{\rm s}},\qquad (4)$$

where ρ_{Rd} is the vapour density near the droplet surface (outside the Knudsen layer). This equation have been derived under the assumption that $\beta_m = 1$.

For arbitrary $\beta_{\rm m}$ the value of $j_{\rm lg}$ can be obtained via the replacement of $\rho_{\rm s}$ in Eq. (4) by [46,50]:

$$\rho_0 = \left(1 - 2\sqrt{\pi} \frac{j_{\rm lg}}{\rho_{\rm s} \sqrt{2R_{\rm g}T_{\rm s}}} \frac{1 - \beta_{\rm m}}{\beta_{\rm m}}\right) \rho_{\rm s}.$$
(5)

The solution of the system of Eqs. (4) and (5) with two unknowns j_{lg} and ρ_0 would allow us to find the required value of j_{lg} for arbitrary $\beta_m \leq 1$. In the limit of weak evaporation $(\rho_s - \rho_{Rd})/\rho_s \ll 1$. Eq. (4) reduces to Eq. (3) for $\beta_m = 1$ (see Appendix A).

3. Basic equations and approximations

The kinetic evaporation model used in the paper is based on Eq. (3) in the case of weak evaporation and on Eqs. (4) and (5) in the case of strong evaporation.

It is assumed that fuel vapour, leaving the Knudsen layer, should be removed from the outer boundary of this layer via diffusion. Thus the mass flux of fuel vapour leaving the droplets is assumed to be equal to the diffusion mass flux from the outer boundary of the Knudsen layer j_{diff} . The condition $j_{\text{lg}} = j_{\text{diff}}$ allows us to determine the value of the mass fraction of fuel vapour at the outer boundary of the Knudsen layer (Y_{fRd}). This equation is solved under the assumption that $T_{\text{Rd}} = T_{\text{s}}$. The value of Y_{fRd} is less or equal to the saturated value Y_{fs} .

The value of j_{diff} is determined from the conventional hydrodynamic theory as:

$$j_{\text{diff}} = \frac{\rho_{\text{mix}} D_{\text{c}}}{R_{\text{d}}} \ln(1 + B_{\text{M}}), \tag{6}$$

where ρ_{mix} is the density of the mixture of gas (air) and fuel vapour at the outer boundary of the Knudsen layer $(\rho_{\text{mix}} = \rho_{\text{Rd}}/Y_{\text{fRd}})$, D_{c} is the binary diffusion coefficient, $B_{\text{M}} = Y_{\text{fRd}}/(1 - Y_{\text{fRd}})$ is the Spalding number.

The values of β_m for diesel fuel are not known at the moment. Their experimental or theoretical estimate have not been performed to the best of our knowledge. Our calculations will be based on two typical values of $\beta_m = 0.5$ and $\beta_m = 0.04$. The first value corresponds to the average experimentally measured value of β_m for water; the second value corresponds to the minimal observed value of β_m for water [19,20].

The hydrodynamic evaporation model used in our analysis is the conventional one (see e.g. [2,5]). Assuming that vapour concentration near the droplet surface is maintained at the saturation level, the evaporation process is controlled by the diffusion of fuel vapour from the droplet surface described by Eq. (6), but with Y_{fRd} replaced by Y_{fs} , where Y_{fs} is the mass fraction of fuel vapour near the droplet surface:

$$Y_{\rm fs} = \left[1 + \left(\frac{p}{p_{\rm s}} - 1\right)\frac{M_{\rm a}}{M_{\rm f}}\right]^{-1},\tag{7}$$

p and p_s are ambient pressure and the pressure of saturated fuel vapour corresponding to droplet surface temperature T_s respectively, M_a and M_f are molar masses of air and fuel; p_s can be calculated from the Clausius–Clapeyron equation presented in the form [5]:

$$p_{\rm s} = \exp\left[a_{\rm f} - \frac{b_{\rm f}}{T_{\rm s} - 43}\right],\tag{8}$$

 $a_{\rm f}$ and $b_{\rm f}$ are constants to be specified for specific fuels, $T_{\rm s}$ is the surface temperature of fuel droplets in K; $p_{\rm s}$ predicted by Eq. (8) is in kPa. The quantity $\rho_{\rm mix}D_{\rm c}$ in Eq. (6) can be replaced by $k_{\rm mix}/c_{\rho(\rm mix})$ assuming that the Lewis number is unity ($Le = k_{\rm mix}/(\rho_{\rm mix}c_{\rho(\rm mix})D_{\rm c}) = 1$). The generalization of this model was discussed in [3].

Heat supplied to the droplet in both kinetic and hydrodynamic models is estimated as [2]:

$$Q = 4\pi R_{\rm d}^2 h (T_{\infty} - T_{\rm s}), \tag{9}$$

where h is obtained from the equation:

$$h = \frac{k_{\rm mix}}{R_{\rm d}} \frac{\ln\left(1 + B_{\rm M}\right)}{B_{\rm M}}.$$
(10)

In the kinetic model $B_{\rm M}$ is defined via $Y_{\rm fRd}$, while in the hydrodynamic model it is defined via $Y_{\rm fs}$.

The heat used for evaporation is

$$Q_{\rm e} = 4\pi R_{\rm d}^2 j_{\rm lg} L,\tag{11}$$

where L is the specific latent heat of evaporation. Ignoring the temperature gradient inside the droplet, the temperature of the latter is found from the equation:

$$\frac{dT_{\rm d}}{dt} = \frac{3}{c_{\rm l}\rho_{\rm l}} [h(T_{\infty} - T_{\rm s}) - j_{\rm lg}L].$$
(12)

The evolution of droplet radius is found from the equation:

$$\frac{\mathrm{d}R_{\mathrm{d}}}{\mathrm{d}t} = -\frac{j_{\mathrm{lg}}}{\rho_{\mathrm{l}}}.$$
(13)

4. Results

. -

The kinetic and hydrodynamic models, described in Section 3, were applied to modelling of heating and evaporation processes of typical fuel droplets in diesel engines. Eq. (3), describing weak evaporation, was used in our calculations. This approximation was justified by the predicted results: the values of drift vapour velocities were much less than the velocity of sound. The gas pressure and the initial droplet temperature were taken equal to 30 bar and 300 K respectively. The effects of temperature gradients inside droplets were ignored (see [66,67] for the discussion of this approximation). In the kinetic model two values of β_m were used: $\beta_m = 0.5$ and $\beta_{\rm m} = 0.04$. These are the average and minimal values of $\beta_{\rm m}$ measured for water [19,20]. The value of $\beta_{\rm m} = 0.04$ is close to $\beta_{\rm m} = 0.06$ estimated by Shusser et al. [68] for butane. As mentioned earlier, the values of β_m for diesel fuel have not been measured or estimated to the best of our knowledge.

Firstly, the heating and evaporation of large droplets with radii 20 μ m were considered. The ambient gas temperature was taken equal to 750 K. This is a typical gas temperature at the end of compression stroke in diesel engines [10]. The results of calculations of droplet temperature and radius, based on hydrodynamic and kinetic models, are shown in Fig. 1. As follows from this figure, kinetic effects lead to a small increase of evaporation time and droplet temperature for $\beta_m = 0.5$. This increase becomes slightly larger for smaller β_m . The overall shapes of the curves diameter versus time, as predicted by hydrodynamic and kinetic models, appear to be rather similar.

In Fig. 2 the results of calculations similar to those presented in Fig. 1, but for the ambient gas temperature equal to 2000 K, are shown. This temperature is a typical gas temperature in diesel engines, after the start of ignition [10]. Hence, Fig. 2 describes the heating and evaporation of fuel droplets injected directly into the flame. This situation is extreme rather than typical for realistic diesel engines conditions [7]. As follows from Fig. 2, the kinetic effects lead to essentially the same



Fig. 1. Plots of droplet temperature (in K) and droplet radius (in μ m) versus time for ambient gas pressure 30 bar, ambient gas temperature $T_{\infty} = 750$ K, and initial droplet radius $R_{d0} = 20$ μ m calculated based on hydrodynamic and kinetic models with the evaporation coefficients $\beta_m = 0.5$ and 0.04.



Fig. 2. The same as Fig. 1 but for $T_{\infty} = 2000$ K.

changes in droplet temperature and diameter as when the ambient gas temperature is equal to 750 K, although the overall evaporation time is about four times less for $T_{\infty} = 2000$ K than for $T_{\infty} = 750$ K. Comparing Figs. 1 and 2 one can see that the relative changes of droplet temperature and diameter due to kinetic effects are noticeably larger for $T_{\infty} = 2000$ K than for $T_{\infty} = 750$ K. In contrast to the case of $T_{\infty} = 750$ K, the dependence of kinetic corrections on β_m is rather small for $T_{\infty} = 2000$ K. These corrections lead to about 6% increase of evaporation time for both β_m for $T_{\infty} = 2000$ K.

In Figs. 3 and 4 the results of calculations similar to those presented in Figs. 1 and 2, but for the initial droplet radius equal to 5 μ m are shown. Droplets with this initial radius are most likely to be observed in diesel engines [6]. As can be seen from these figures, for both temperatures $T_{\infty} = 750$ K and $T_{\infty} = 2000$ K the kinetic effects lead to the same increase of evaporation times



Fig. 3. The same as Fig. 1 but for $R_{d0} = 5 \ \mu m$.



Fig. 4. The same as Fig. 2 but for $R_{d0} = 5 \ \mu m$.

and droplet temperature as for a droplet with an initial droplet radius equal to 20 µm (cf. Figs. 1 and 2). For small droplets these effects are noticeably stronger than for large droplets, as expected. Also, for smaller droplets, the increase of droplet temperature and evaporation time with decreasing β_m is clearly visible, especially for $T_{\infty} = 750$ K. For $T_{\infty} = 750$ K and $\beta_{\rm m} = 0.04$ the kinetic model predicts about 6% longer evaporation time than the hydrodynamic model. For $T_{\infty} = 2000$ K and $\beta_{\rm m} =$ 0.04 the predicted evaporation time becomes about 9% longer than predicted by the hydrodynamic model. This increase of evaporation time should be taken into account when modelling the evaporation of fuel droplets in realistic diesel engines. The increase of droplet evaporation time would lead to an increase to the physical ignition delay and to the overall ignition delay in diesel engines [10]. This would affect the timing of the autoignition-the crucial parameter for the performance of these engines [6]. As in the case of large droplets, for droplets with the initial diameter 5 µm the ambient gas temperature leads to relatively weak effects on the increase of evaporation time and droplet temperature predicted by the kinetic model. As expected, the increase of ambient gas temperature from 750 to 2000 K leads to a decrease of the evaporation time by a factor of four.

The results for $T_{\infty} = 2000$ K are shown mainly to illustrate the general trends of the process at high temperature. The quantitative results could have limited reliability, as at this temperature, the mean free path of molecules can be comparable with the molecular diameters. As mentioned earlier, in this situation we approach the limit of applicability of Boltzmann equation. To the best of our knowledge, nobody ever attempted to analyse this problem using the Bogolubov–Born–Green– Kirkwood–Ivon hierarchy of equations [69]. This would have been the only way to solve the problem without the abovementioned limitation on *l*.

The results of calculations similar to the ones presented above but for atmospheric pressure showed that a decrease of pressure from 30 atm to 1 atm leads to a substantial increase in contribution from kinetic effects. Also, the dependence of the evaporation time on β_m appears to be much more pronounced for 1 atm than for 30 atm. In particular, for $T_{\infty} = 750$ K, $R_{d0} = 5 \ \mu m$ and $\beta_m = 0.04$ the kinetic model predicts about 30% longer evaporation time than the hydrodynamic model.

The kinetic effects appear to be even more pronounced for droplets with an initial radius of 1 μ m. In this case, however, our model appears to be less reliable, as it does not take into account the effects of surface tension. For droplets with this initial radius these effects are expected to be noticeable.

5. Conclusions

A comparative analysis of hydrodynamic and kinetic approaches to the problem of diesel fuel droplet evaporation has been presented. The hydrodynamic approach is based on the assumption that the concentration of fuel vapour near the droplet surface is maintained at saturation level. This approach is universally used in computational fluid dynamics (CFD) codes. In the kinetic approach the mass flow rate of fuel vapour from the droplet surface is calculated based on the solution of the Boltzmann equation for given evaporation coefficients β_m . The mass flow rate of fuel vapour as predicted by the kinetic model has been calculated from Eq. (3) (weak evaporation). Two values of the evaporation coefficient have been used $\beta_m = 0.5$ and $\beta_{\rm m} = 0.04$. These are the average and minimal values of $\beta_{\rm m}$ measured for water. The values of $\beta_{\rm m}$ for diesel fuel have not been measured or estimated to the best of our knowledge. It is pointed out that the kinetic effects on droplet evaporation are always noticeable, despite the fact that this evaporation takes place at rather high pressures (up to 30 atm and even more). This shows the limitation of the applicability of the hydrodynamic approach to accurate modelling of this processes. As expected, kinetic models predict longer evaporation time and higher droplet temperature compared with the hydrodynamic model. The kinetic effects are shown to be more pronounced for smaller droplets (5 μ m) than for larger ones (20 μ m). The droplet evaporation time and droplet temperature increase with decreasing evaporation coefficient. It is recommended that the kinetic effects are taken into account when modelling the evaporation process of diesel fuel droplets in realistic internal combustion engines.

Acknowledgements

The authors are grateful to the Royal Society for partial financial support of this project in the form of a Travel Grant. One of the authors (SSS) is grateful to Professor I Shreiber (Ben-Gurion University, Israel) for stimulating discussions of the kinetic models of droplets evaporation. These discussions were the main driving force behind the idea of preparation of this paper.

Appendix A

Assuming that $(\rho_s - \rho_{\rm Rd})/\rho_s \equiv N_\rho \ll 1$ (weak evaporation), we can write:

$$\sqrt{\frac{\rho_{\rm Rd}}{\rho_{\rm s}}}(\rho_{\rm s}-\rho_{\rm Rd})=N_{\rho}\rho_{\rm s}.\tag{A.1}$$

Using Equation (2.27) of [50] we obtain, remembering that $N_{\rho} \ll 1$:

$$\frac{T_{\rm s} - T_{\rm Rd}}{T_{\rm s}} \equiv N_{\rm T} = 0.265 \frac{\rho_{\rm s} - \rho_{\rm Rd}}{\rho_{\rm s} \sqrt{\rho_{\rm Rd}/\rho_{\rm s}}} = 0.265 N_{\rho}.$$
 (A.2)

Using the gas law and ignoring non-linear terms the following relation is obtained:

$$p_{\rm s} - p_{\rm Rd} = p_{\rm s}(N_{\rm T} + N_{
ho}).$$
 (A.3)

Eqs. (A.2) and (A.3) allow us to rewrite Eq. (A1) as:

$$\sqrt{\frac{\rho_{\rm Rd}}{\rho_{\rm s}}}(\rho_{\rm s}-\rho_{\rm Rd}) = \rho_{\rm s}\frac{N_{\rm T}+N_{\rho}}{1.265} = \rho_{\rm s}\frac{p_{\rm s}-p_{\rm Rd}}{1.265p_{\rm s}}.$$
 (A.4)

Having substituted Eq. (A4) into Eq. (4) we obtain:

$$j_{lg} = 0.6\sqrt{2R_gT_s}\rho_s \frac{p_s - p_{Rd}}{1.265p_s} = \frac{1.2\sqrt{\pi}}{1.265} \frac{\rho_s R_g T_s(p_s - p_{Rd})}{p_s\sqrt{2\pi R_gT_s}}$$
$$= 1.681 \frac{p_s - p_{Rd}}{\sqrt{2\pi R_gT_s}}$$

This expression differs by less than 1% from Eq. (3) taken for $\beta_m = 1$.

References

- J.S. Chin, A.H. Lefebvre, Steady-state evaporation characteristics of hydrocarbon fuel drops, AIAA J. 21 (1983) 1437–1443.
- [2] A.H. Lefebvre, Atomization and Sprays, Taylor & Francis, 1989.
- [3] B. Abramzon, W.A. Sirignano, Droplet vaporization model for spray combustion calculations, Int. J. Heat Mass Transfer 32 (1989) 1605–1618.
- [4] S.K. Aggarwal, A review of spray ignition phenomena: present status and future research, Prog. Energy Combust. Sci. 24 (1998) 565–600.
- [5] W.A. Sirignano, Fluid Dynamics and Transport of Droplets and Sprays, Cambridge University Press, 1999.
- [6] P.F. Flynn, R.P. Durrett, G.L. Hunter, A.O. zur Loye, O.C. Akinyemi, J.E. Dec, C.K. Westbrook, Diesel combustion: an integrated view combining laser diagnostics, chemical kinetics, and empirical validation, SAE Report 1999-01-0509, 1999.
- [7] R.Z. Kavtaradze, Local Heat Transfer in Reciprocating Engines, Moscow State Technical Bauman University Publishing House, 2001 (in Russian).
- [8] G. Miliauskas, Interaction of the transfer processes in semitransparent liquid droplets, Int. J. Heat Mass Transfer 46 (2003) 4119–4138.
- [9] S.S. Sazhin, G. Feng, M.R. Heikal, I. Goldfarb, V. Goldshtein, G. Kuzmenko, Thermal ignition analysis of a monodisperse spray with radiation, Combust. Flame 124 (2001) 684–701.
- [10] E.M. Sazhina, S.S. Sazhin, M.R. Heikal, V.I. Babushok, R. Johns, A detailed modelling of the spray ignition process in Diesel engines, Combust. Sci. Technol. 160 (2000) 317–344.
- [11] S.V. Utyuzhnikov, Numerical modeling of combustion of fuel-droplet-vapour releases in the atmosphere, Flow Turbul. Combust. 68 (2002) 137–152.
- [12] M. Burger, R. Schmehl, K. Prommersberger, O. Schäfer, R. Koch, S. Wittig, Droplet evaporation modelling by the distillation curve model: accounting for kerosene fuel and elevated pressure, Int. J. Heat Mass Transfer 46 (2003) 4403–4412.
- [13] H. Hertz, Über die Verdunstung der Flussigkeiten, inbesondere des Quecksilbers, im lufteeren Raume, Ann. Phys. Chem. 17 (1882) 177–200.
- [14] M. Knudsen, Die Maximale Verdampfungsgeschwindigkeit des Quecksilbers, Ann. Phys. Chem. 47 (1882) 697–708.
- [15] R.W. Schrage, A Theoretical Study of Interface Mass Transfer, Columbia University Press, New York, 1953.
- [16] M.N. Kogan, Rarefied Gas Dynamics, Plenum, New York, 1969.
- [17] V.P. Shidlovskiy, Introduction to the Dynamics of Rarefied Gases, American Elsevier Publishing Company, New York, 1967.
- [18] R.I. Nigmatilin, in: Dynamics of Multiphase Media, vol. 1, Hemisphere Publishing Corporation, 1991.

- [19] J.P. Hirth, G.M. Pound, Condensation and Evaporation. Nucleation and Growth Kinetics, Pergamon Press, Oxford, London, Paris, Frankfurt, 1963.
- [20] A.I. Neizvestny, L.I. Onishenko, Experimental determination of the condensation coefficient for distilled water, Phys. Atmos. Ocean 15 (1979) 1052–1078 (in Russian).
- [21] T. Tsuruda, H. Tanaka, T. Masuika, Condensation/evaporation coefficient and velocity distribution at liquid– vapour interface, Int. J. Heat Mass Transfer 42 (1999) 4107–4116.
- [22] D.O. Dunikov, S.P. Malyshenko, V.V. Zhakhovskii, Corresponding states law and molecular-dynamics simulations of the Lennard–Jones fluid, J. Chem. Phys. 115 (2001) 6623–6631.
- [23] L. Consoline, S.K. Aggarwal, S. Murad, A molecular dynamics simulation of droplet evaporation, Int. J. Heat Mass Transfer 43 (2003) 3179–3188.
- [24] N.A. Gumerov, Dynamics of vapour bubbles with nonequilibrium phase transitions in isotropic acoustic fields, Phys. Fluids 12 (2000) 71–88.
- [25] Y. Sone, H. Sugimoto, Strong evaporation from a plane condensed phase, in: G.E.A. Meier, P.A. Thompson (Eds.), Adiabatic Waves in Liquid–Vapour Systems, Proc. IU-TAM Symposium, Gottingen, Germany, 1989, Springer-Verlag, Berlin, 1990, pp. 293–304.
- [26] E.M. Lifshitz, L.P. Pitaevski, Physical Kinetics, Nauka Publishing House, Moscow, 1979.
- [27] R.Ya. Kucherov, L.E. Rickenglaz, On hydrodynamics boundary conditions for modelling vaporization and condensation processes, J. Exp. Theor. Phys. 37 (1959) 125– 126 (in Russian).
- [28] R.Ya. Kucherov, L.E. Rickenglaz, On the measurement of the coefficient of condensation, Rep. Acad. Sci. USSR (Doklady) 133 (1960) 1130–1131 (in Russian).
- [29] R.Ya. Kucherov, L.E. Rickenglaz, T.S. Tzulaya, Kinetic theory of additional condensation in the presence of the small temperature jump, Soviet Phy.—Tech. Phys. 7 (1963) 1027–1030.
- [30] D.A. Labuntsov, Analysis of the evaporation and condensation processes, High Temp. 5 (1967) 579–585.
- [31] T.M. Muratova, D.A. Labuntsov, Kinetic analysis of the evaporation and condensation processes, Thermal Phys. High Temp. 7 (1969) 959–967 (in Russian).
- [32] P.L. Bhatnagar, E.P. Gross, M. Krook, A model for collision processes in gases 1. Small amplitude processes in charged and neutral one component systems, Phys. Rev. 94 (1954) 511–525.
- [33] S.S. Sazhin, in: Cyclotron whistler-mode instability in a collisional plasma, Geomagnetic Research, No. 23, Soviet Radio, Moscow, 1978, pp. 105–107 (in Russian).
- [34] A.V. Korabelnikov, V.E. Nakoryakov, I.R. Shreiber, Taking nonequilibrium vaporization into account in problems of vapour-bubble dynamics, High Temp. 19 (1981) 586–590.
- [35] P. Young-ping-Pao, Application of kinetic theory to the problem of evaporation and condensation, Phys. Fluids 14 (1971) 306–311.
- [36] Y. Sone, Y. Onishi, Kinetic theory of evaporation and condensation, J. Phys. Soc. Jpn. 35 (1973) 1773–1776.

- [37] Y. Sone, Y. Onishi, Kinetic theory of evaporation and condensation—hydrodynamic equation and slip boundary condition, J. Phys. Soc. Jpn. 44 (1978) 1981–1994.
- [38] J.W. Cipola, J.H. Lang, S.K. Loyalka, Kinetic theory of evaporation and condensation, Proceedings of 8th International Symposium on Rarefied Gas Dynamics, New York–London, 1973, pp. 1773–1776.
- [39] J.R. Thomas, T.S. Chang, S.E. Siewert, Reverse temperature gradient in the kinetic theory of evaporation, Phys. Rev. Lett. 33 (1974) 680–682.
- [40] P.N. Shankar, F.M. Marble, Kinetic theory of transient condensation and evaporation at a plane surface, Phys. Fluids 14 (1971) 510–516.
- [41] L.D. Koffman, M.S. Plesset, L. Lees, Theory of evaporation and condensation, Phys. Fluids 27 (1984) 876–880.
- [42] T. Ytrehus, T Aukrust, Mott–Smith solution for weak condensation, in: V. Boffi, C. Cercignani (Eds.), Rarefied Gas Dynamics, vol. 2, Teubner, Stuttgart, 1986, pp. 271– 280.
- [43] V. Chernyak, The kinetic theory of droplet evaporation, J. Aerosol. Sci. 26 (1995) 873–885.
- [44] S.I. Anisimov, Evaporation of metals under the influence of laser radiation, J. Exp. Theor. Phys. 54 (1968) 339–342 (in Russian).
- [45] S.I. Anisimov, Ya.A. Imas, G.S. Romanov, Yu.V. Khodyko, Effect of high intensity radiation on metals, Nauka Publishing House, Moscow, 1970 (in Russian).
- [46] M.N. Kogan, N.K. Makashev, On the role of the Knudsen layer in the theory of heterogeneous reactions and flows with the surface reactions, Reports of the Academy of Sciences of USSR: Mechanics of Liquids and Gases, No. 6, 1971, pp. 3–11 (in Russian).
- [47] M. Murakami, K. Oshima, Kinetic approach to the transient evaporation and condensation problem, in: M. Becker, M. Fiebig (Eds.), Rarefied Gas Dynamics, DFVLR Press, Pors-Wahn, 1974, paper F6.
- [48] T. Ytrehus, Theory and experiments on gas kinetics in evaporation, in: J.L. Potter (Ed.), Rarefied Gas Dynamics Part 2, AIAA, New York, 1977, pp. 1197–1212.
- [49] D.A. Labuntsov, A.P. Kryukov, Processes of intensive evaporation, Thermal Power Energy (Teploenergetika 4) (1977) 8–11 (in Russian).
- [50] D.A. Labuntsov, A.P. Kryukov, Analysis of intensive evaporation and condensation, Int. J. Heat Mass Transfer 22 (1979) 989–1002.
- [51] S.J. Knight, Theoretical modelling of rapid surface vaporization with back pressure, AIAA. J. 17 (1979) 519– 523.
- [52] C. Cercignani, Strong evaporation of a poliatomic gas, in: S.S. Fisher (Ed.), Rarefied Gas Dynamics Part 2, AIAA, New York, 1981, pp. 305–310.
- [53] A.A. Abramov, M.N. Kogan, N.K. Makashev, Numerical analysis of the processes in strongly non-equilibrium Knudsen layers, Reports of the Academy of Sciences of USSR: Mechanics of Liquids and Gases, No. 3, 1981, pp. 72–81 (in Russian).
- [54] A. Frezzotti, Kinetic theory study of the strong evaporation of a binary mixture, in: V. Boffi, C. Cercignani (Eds.), Rarefied Gas Dynamics, vol. 2, Teubner, Stuttgart, 1986, pp. 313–322.

- [55] Y. Sone, K. Aoki, H. Sugimoto, T. Yamada, Steady evaporation and condensation on a plane condensed phase, Theor. Appl. Mech. (Bulgaria) 19 (1988) 89– 93.
- [56] T. Ytrehus, S. Ostmo, Kinetic approach to interface processes, Int. J. Multiphase Flow 22 (1996) 133–135.
- [57] S. Takata, K. Aoki, Two-surface problems of a multicomponent mixture of vapors and noncondensable gases in the continuum limit in the light of kinetic theory, Phys. Fluids 11 (1999) 2743–2756.
- [58] D. Sibold, H.M. Urbassek, Kinetic study of evaporating flows from cylindrical jets, Phys. Fluids 3 (1991) 870– 878.
- [59] H. Sugimoto, Y. Sone, Numerical analysis of steady flows of a gas evaporating from its cylindrical condensed phase on the basis of kinetic theory, Phys. Fluids 4 (1992) 419– 440.
- [60] Y. Sone, H. Sugimoto, Kinetic theory analysis of steady evaporating flows from a spherical condensed phase into a vacuum, Phys. Fluids 5 (1993) 1491–1511.
- [61] Y. Sone, H. Sugimoto, Evaporation of rarefied gas from a cylindrical condensed phase into a vacuum, Phys. Fluids 7 (1995) 2072–2085.
- [62] Y. Sone, H. Sigimoto, K. Aoki, Cylindrical Couette flows of a rarefied gas with evaporation and condensation: reversals and bifurcation of flows, Phys. Fluids 11 (1999) 476–490.

- [63] Y. Sone, Kinetic theoretical studies of the half-space problem of evaporation and condensation, Transport Theory Stat. Phys. 29 (2000) 227–260.
- [64] V.A. Titarev, E.M. Shahov, Heat loss and evaporation from a flat surface after a rapid increase of its temperature, Reports of the Russian Academy of Sciences: Mechanics of Liquids and Gases, No. 1, 2002, pp. 141–153 (in Russian).
- [65] J. Rose, Interphase matter transfer, the condensation coefficient and dropwise condensation. In: Proceedings of 11th International Heat Transfer Conference, 23–28 August 1998, Kyongji, Korea, vol. 1, 1998, pp. 89–104.
- [66] C. Bertoli, M. Migliaccio, A finite conductivity model for diesel spray evaporation computations, Int. J. Heat Fluid Flow 20 (1999) 552–561.
- [67] S.S. Sazhin, P.A. Krutitskii, A conduction model for transient heating of fuel droplets, in: H.G.W. Begehre, R.P. Gilbert, M.W. Wong (Eds.), Progress in Analysis, Proceedings of the 3rd International ISAAC (International Society for Analysis, Applications and Computations) Congress, 20–25 August 2001, Berlin, vol. II, World Scientific, Singapore, 2003, pp. 1231–1239.
- [68] M. Shusser, T. Ytrehus, D. Weihs, Kinetic theory analysis of explosive boiling of a liquid droplet, Fluid Dynam. Res. 27 (2000) 353–367.
- [69] A.I. Akhiezer, I.A. Akhiezer, P.V. Polovin, A.G. Sitenko, K.N. Stepanov, Plasma Electrodynamics, Nauka Publishing House, Moscow, 1974 (in Russian).