

NEW APPROACHES TO MODELLING DROPLET HEATING AND EVAPORATION

S.S. Sazhin*, I.G. Gusev*, J.-F. Xie*, A.E. Elwardany*, A.Yu. Snegirev^o, M.R. Heikal*¹

*Sir Harry Ricardo Laboratories, School of Computing, Engineering and Mathematics,
University of Brighton, Brighton BN2 4GJ, U.K.

^oSaint-Petersburg State Polytechnic University, Polytechnicheskaya, 29, Saint-Petersburg 195251, Russia.

¹Current address: Department of Mechanical Engineering, Universiti of Teknologies PETRONAS, Bandar Sri
Iskandar 31750 Tronoh, Perak Darul Ridzuan, Malaysia

ABSTRACT

New solutions to the droplet heat conduction equation, assuming that the droplet radius is a linear function of time, are described alongside new solutions to the same equation, assuming that the time evolution of droplet radius $R_d(t)$ is known. For sufficiently small time steps the time evolutions of droplet surface temperatures and radii, predicted by both approaches for typical Diesel engine-like conditions, coincide. Both solutions predict lower droplet temperatures and slower evaporation when the effects of the reduction of $R_d(t)$ due to evaporation are taken into account. A simplified model for multi-component droplet heating and evaporation, based on an analytical solution to the species diffusion equation, is discussed. This model has been generalised to take into account the effect of coupling between the droplets and the surrounding gas. A new approach to modelling multi-component droplets, including large numbers of components, heating and evaporation is discussed. This new approach is based on the replacement of a large number of actual components with a small number of quasi-components. The evaporation and condensation of n-dodecane ($C_{12}H_{26}$) are investigated using the molecular dynamics (MD) simulation technique. The values of the evaporation/condensation coefficient are estimated.

INTRODUCTION

In most commercial and research computational fluid dynamics (CFD) codes the modelling of droplet heating and evaporation is based on the assumptions that: there is no temperature gradient inside droplets; the droplet radius is fixed during each time step, although it changes from one time step to another; kinetic effects can be ignored; and in the case of multi-component droplets, the species diffusivity within the droplet is infinitely large or small [1].

The aim of this paper is to summarise some of the most recent developments in the modelling of droplet heating and evaporation processes, in which the above mentioned commonly used assumptions are relaxed. For mono-component droplets, these models take into account the effect of finite thermal conductivity and recirculation in the moving droplets, alongside the change in droplet radius during individual time steps [2,3]. For multi-component droplets, including relatively small numbers of components, the new models are based on the analytical solution of the species diffusion equation inside the droplet [4,5]. The model designed to take into account large numbers of components is based on the introduction of the concept of quasi-components [6]. A new approach to calculating the evaporation coefficient of n-dodecane, the closest approximation to Diesel fuel, is described based on [7]. This coefficient is essential for the accurate kinetic modelling of droplet evaporation.

The paper will start with an overview of results referring to hydrodynamic models of mono-component droplets, after which the modelling of multi-component droplets with small and large numbers of components is discussed. Then the focus moves to kinetic modelling with particular emphasis on calculation of the evaporation/condensation coefficient. Finally the conclusions of the paper are drawn.

MONO-COMPONENT DROPLETS: HYDRODYNAMIC MODELS

Assuming that droplet heating is spherically symmetric, the transient heat conduction equation inside droplets can be written as [1]:

$$\frac{\partial T}{\partial t} = \frac{\kappa}{R^2} \frac{\partial}{\partial R} \left(R^2 \frac{\partial T}{\partial R} \right) + P(t, R), \quad (1)$$

where $\kappa = k_l / (c_l \rho_l)$ is the liquid thermal diffusivity, k_l , c_l , and ρ_l are the liquid thermal conductivity, specific heat capacity, and density, respectively, R is the distance from the centre of the spherical droplet, t is time. The boundary and initial conditions for this equation, ignoring the effect of evaporation, can be presented as:

$$h(T_g - T_s) = k_l \frac{\partial T}{\partial R} \Big|_{R=R_d}, \quad (2)$$

$$T(t=0) = T_{d0}(R), \quad (3)$$

where $T_s = T_s(t)$ is the droplet's surface temperature, $T_g = T_g(t)$ is the ambient gas temperature, $h = h(t)$ is the convective heat transfer coefficient, linked with the Nusselt number Nu via the equation $Nu = 2R_d h / k_g$, k_g is the gas thermal conductivity. To take into account the effect of evaporation the gas temperature T_g is replaced by the so-called effective temperature T_{eff} [1]:

$$T_{eff} = T_g + \rho_l L \frac{dR_d}{dt} / h, \quad (4)$$

where L is the latent heat of evaporation and $\frac{dR_d}{dt}$ is the rate of change of droplet radius due to evaporation.

In the case when the convection heat transfer coefficient $h(t) = h = \text{const}$, the solution to the transient heat conduction equation (1), with $R_d = \text{const}$ and the corresponding boundary (2) and initial (3) conditions, can be presented as [1]:

$$T = T_{\text{eff}} + \frac{R_d}{R} \sum_{n=1}^{\infty} \left\{ \left[q_n - \frac{\sin \lambda_n \mu_0(0)}{\lambda_n^2 \|V_n\|^2} \right] \exp(-\kappa_0 \lambda_n^2 t) - \frac{\sin \lambda_n}{\lambda_n^2 \|V_n\|^2} \int_0^1 \frac{d\mu_0(\tau)}{d\tau} \exp[-\kappa_0 \lambda_n^2 (t - \tau)] d\tau \right\} \sin\left(\frac{\lambda_n R}{R_d}\right) + \frac{R_d}{R} \sum_{n=1}^{\infty} \frac{p_n}{\kappa_0 \lambda_n^2} \left[1 - \exp(-\kappa_0 \lambda_n^2 t) \right] \sin\left(\frac{\lambda_n R}{R_d}\right). \quad (5)$$

A set of positive eigenvalues λ_n , numbered in ascending order ($n=1, 2, \dots$) (the trivial solution $\lambda = 0$ is not considered), is found from the solution of the following equation:

$$\lambda_n \cos \lambda_n + h_0 \sin \lambda_n = 0, \quad (6)$$

$$h_0 = \frac{hr_d}{k_l} - 1, \quad \|V_n\|^2 = 0.5(1 - \sin 2\lambda_n / 2\lambda_n),$$

$$V_n = \sin(\lambda_n R / R_d),$$

$$\kappa_0 = k_l / (c_l \rho_l R_d^2),$$

$$p_n = \frac{1}{\|V_n\|^2} \int_0^1 \left[\frac{RP(t, R)}{R_d} \right] V_n(R) d(R / R_d).$$

The generalisation of the above model to the case of moving droplets (Effective Thermal Conductivity (ETC) model) can be achieved by replacing the thermal conductivity of liquid k_l with the effective thermal conductivity $k_{\text{eff}} = \chi k_l$, where the coefficient χ varies from about 1 (at droplet Peclet numbers < 10) to 2.72 (at droplet Peclet numbers > 500). The variations of all parameters with temperature and time were accounted for when analytical solution (4) was incorporated into a numerical code.

This model was applied to the modelling of droplet heating and evaporation, assuming that droplet radius remains constant during the time step. Assuming that the Lewis number is equal to 1, the change of the droplet radius from one time step to another was described by the following equation [2]:

$$\frac{dR_d}{dt} = - \frac{k_g \text{Sh}}{2\rho_l c_{pg} R_d}, \quad (7)$$

where k_g is the gas thermal conductivity, c_{pg} is the gas specific heat capacity at constant pressure, Sh is the Sherwood number. When solving Equation (7) it was assumed that the temperature remained the same during the time step.

Solution (5) has been generalised to the case when droplet radius was assumed to be a linear function during the time step [2] or an arbitrary

function $R_d(t)$ [3]. In the latter case, the solution turned out to be the simplest when the initial droplet temperature is assumed to be constant. Since $R_d(t)$ depends on the time evolution of the droplet temperature, an iterative process is required. Firstly, the time evolution of $R_d(t)$ is obtained using the conventional approach, when it remains constant during the time step, but changes from one time step to another. Then these values of $R_d(t)$ are used in the new solutions to obtain updated values of the time evolution of the distribution of temperatures inside the droplet and on its surface. These new values of droplet temperature are used to update the function $R_d(t)$. This process continues until convergence is achieved, which typically takes place after about 15 iterations. The results of these calculations were compared with the results obtained using the approach when the droplet radius was assumed to be a linear function of time during individual time steps for typical Diesel engine-like conditions. For sufficiently small time steps the time evolutions of droplet temperatures and radii predicted by both approaches coincided. This suggests that both approaches are correct and valid. Similarly to the case when droplet radius is assumed to be a linear function of time during the time step, the solutions for arbitrary $R_d(t)$ predict lower droplet temperature and slower evaporation when the effects of the reduction of $R_d(t)$ are taken into account. It is shown that in the case of constant droplet initial temperature, models both taking and not taking into account the changes in the initial droplet temperature with the distance from the droplet centre predict the same results. This indicates that both models are correct. The correctness of this approach is further supported by agreement between the results obtained in [2] and those reported in [8]. In the latter paper the analysis is based on the direct numerical solution to Equation (1), taking into account the effect of the moving boundary.

MULTI-COMPONENT DROPLETS: HYDRODYNAMIC MODELS

For modelling multi-component droplet heating and evaporation, the same equations as used for mono-component droplets are applied, but these are complemented by the equations for species mass fractions ($Y_{li} \equiv Y_{li}(t, R)$) inside the droplets [1]:

$$\frac{\partial Y_{li}}{\partial t} = D_l \left(\frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right), \quad (8)$$

where $i > 1$, D_l is the liquid mass diffusivity. Equation (8) is solved subject to the boundary condition [1]:

$$\alpha(\epsilon_i - Y_{lis}) = -D_l \left. \frac{\partial Y_{li}}{\partial R} \right|_{R=R_d-0}, \quad (9)$$

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

$$\alpha = \frac{|m_d|}{4\pi\rho_l R_d^2}, \quad (10)$$

$\epsilon_i = Y_{vis}/\sum_i Y_{vis}$ are species evaporation rates. The effect of recirculation in the moving droplets is taken into account by replacing D_l with $D_{eff} = \chi_Y D_l$, where χ_Y is determined by Equation (18) of [4]. This model is known as the Effective Diffusivity (ED) model.

In contrast to the previously used models, our approach is based on the analytical solution of Equation (8) subject to the above mentioned boundary and initial conditions [4,5]:

$$\begin{aligned} Y_{li} = \epsilon_i + \frac{1}{R} \left\{ \exp \left[D_l \left(\frac{\lambda_0}{R_d} \right)^2 t \right] [q_{i0} - \epsilon_i(0)Q_0] - \right. \\ Q_0 \int_0^t \frac{d\epsilon_i(\tau)}{d\tau} \exp \left[D_l \left(\frac{\lambda_0}{R_d} \right)^2 (t - \right. \\ \left. \left. \tau) \right] d\tau \right] \sinh \left(\lambda_0 \frac{R}{R_d} \right) + \\ \sum_{n=1}^{\infty} \left[\exp \left[-D_l \left(\frac{\lambda_n}{R_d} \right)^2 t \right] [q_{in} - \epsilon_i(0)Q_n] - \right. \\ \left. Q_n \int_0^t \frac{d\epsilon_i(\tau)}{d\tau} \exp \left[-D_l \left(\frac{\lambda_n}{R_d} \right)^2 (t - \right. \right. \\ \left. \left. \tau) \right] d\tau \right] \sin \left(\lambda_n \frac{R}{R_d} \right) \right\}, \quad (11) \end{aligned}$$

where λ_0 is the non-zero solution of equation $\tanh \lambda = -\lambda/h_{0Y}$, λ_n are the solutions of Equation (6), with h_0 being replaced with h_{0Y} ,

$$\begin{aligned} Q_n = & \begin{cases} -\frac{1}{\|v_0\|^2} \left(\frac{R_d}{\lambda_0} \right)^2 (1 + h_{0Y}) \sinh \lambda_0 & \text{when } n = 0 \\ \frac{1}{\|v_n\|^2} \left(\frac{R_d}{\lambda_n} \right)^2 (1 + h_{0Y}) \sin \lambda_n & \text{when } n \geq 1 \end{cases} \\ \|v_n\|^2 = & \begin{cases} \frac{R_d}{2} \left[1 + \frac{h_{0Y}}{h_{0Y}^2 - \lambda_0^2} \right] & \text{when } n = 0 \\ \frac{R_d}{2} \left[1 + \frac{h_{0Y}}{h_{0Y}^2 - \lambda_n^2} \right] & \text{when } n \geq 1 \end{cases}, \\ q_{in} = & \begin{cases} \frac{1}{\|v_0\|^2} \int_0^{R_d} R Y_{li0}(R) \sinh \left(\lambda_0 \frac{R}{R_d} \right) dR & \text{when } n = 0 \\ \frac{1}{\|v_n\|^2} \int_0^{R_d} R Y_{li0}(R) \sin \left(\lambda_n \frac{R}{R_d} \right) dR & \text{when } n \geq 1 \end{cases} \\ h_{0Y} = & - \left(1 + \frac{\alpha R_d}{D_l} \right). \end{aligned}$$

The molar fractions of species i in the vapour phase at the droplet surface are determined as:

$$X_{vi} = X_{li} \gamma_i \exp \left[\frac{L_i M_i}{R_u} \left(\frac{1}{T_{bi}} - \frac{1}{T_s} \right) \right], \quad (12)$$

where X_{li} are the liquid molar fractions at the surface of the droplet, γ_i are the activity coefficients. L_i , M_i and T_{bi} are the latent heat of evaporation, molar masses and boiling temperatures of species i , R_u is the universal gas

constant, T_s is the droplet surface temperature. The activity coefficient for the ethanol/acetone mixture has been estimated following [9]. In the limit, when $\gamma_i = 1$ the Raoult law is valid.

The above model has been generalised to take into account the effects of the moving boundaries on the solution to Equation (8) and tested against available experimental data (see [4,5] for details). Two new solutions to the equation, describing the diffusion of species during multi-component droplet evaporation, are described. The first solution is the explicit analytical solution to this equation, while the second one reduces the solution of the differential transient species 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, assuming that this radius is a linear function of time. These solutions can be considered as the generalisations of the solutions reported earlier. The analytical solution is presented in the case when parameter h_{0Y} can be assumed to be a constant, the value of which is less than -1 during the time step. These solutions are complementary to the ones suggested earlier, which took into account the effect of the moving boundary due to droplet evaporation on the distribution of temperature inside the droplet. The analytical solution has been incorporated into a zero dimensional CFD code and applied to the analysis of bi-component droplet heating and evaporation. The case of an initial 50% ethanol - 50% acetone mixture and droplets with initial diameter equal to 142.7 μm , as in our earlier paper [4], has been considered. Effects of droplets on gas have been ignored at this stage and droplet velocity has been assumed to be constant and equal to 12.71 m/s. To separate the effect of the moving boundary on the species diffusion equation from similar effects on the heat conduction equation inside droplets, described in [4,5], a rather artificial assumption that the droplet temperature is homogeneous and fixed has been made. The moving boundary slows down the increase in the mass fraction of ethanol (the less volatile substance in the mixture) during the evaporation process and accelerates droplet evaporation.

The original simplified model (not taking into account the effects of the moving boundary) has been generalised to take into account the effect of coupling between the droplets and the surrounding gas [5]. The new model has been validated against the observed average droplet temperatures in a monodisperse spray for various n-decane/3-pentanone droplet mixtures. It is concluded that the effect of coupling leads to noticeably better agreement with the experimental results than the results of the one-way solution. The simplified bi-component model has also been implemented into the FLUENT CFD code. Both the stand-alone zero-

dimensional code and FLUENT CFD code predict identical results in identical cases, when the effects of droplets on gas are ignored and gas in the enclosure is assumed to be homogeneous. This opens the way for using the customised version of the FLUENT code, incorporating the new model of bi-component droplet heating and evaporation, for the analysis of realistic cases referring to inhomogeneous enclosures, taking into account the effects of droplets on gas.

The main limitation of this model is that it is able to take into account a rather limited number of components, while realistic fuels usually include a very large number of these components. An alternative model, suggested in [6] is based on replacing the large number of actual components with a small number of quasi-components. These quasi-components are then treated as actual components in the model described earlier, taking into account the diffusion of quasi-components in droplets. The model has been applied to Diesel fuel droplets which have been approximated as a mixture of 21 actual components C_nH_{2n+2} , where $n \geq 5$. These 21 actual components have been replaced by up to 20 quasi-components (the maximal number of quasi-components in this model).

The initial mole fraction of each quasi-component is calculated as:

$$X_j = \int_{n_{j-1}}^{n_j} f_m(n) dn, \quad (13)$$

where j is an integer in the range $1 \leq j \leq N_f$, N_f is the number of quasi-components, $n_0 \leq n \leq n_f$ and $f_m(n)$ is the distribution function approximated as:

$$f_m(n) = C_m(n_0, n_f) \frac{(M(n)-\gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp\left[-\left(\frac{M(n)-\gamma}{\beta}\right)\right], \quad (14)$$

where $M(n) = 14n + 2$ are the molecular weights, $n_0 = 5$, $n_f = 25$, $\Gamma(\alpha)$ is the Gamma function, α and β are parameters that determine the shape of the distribution and γ determines the original shift. We assume that $\alpha = 18.5$, $\beta = 10$ and $\gamma = 0$. The constant $C_m(n_0, n_f)$ is defined as [6]:

$$C_m(n_0, n_f) = \left\{ \int_{n_0}^{n_f} \frac{(M(n)-\gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp\left[-\left(\frac{M(n)-\gamma}{\beta}\right)\right] dn \right\}^{-1}. \quad (15)$$

Each quasi-component has a number of carbon atoms estimated as [6]:

$$\bar{n}_j = \frac{\int_{n_{j-1}}^{n_j} n f_m(n) dn}{\int_{n_{j-1}}^{n_j} f_m(n) dn}. \quad (16)$$

The latent heat and saturation pressure for each quasi-component have been calculated by replacing n with \bar{n}_j . Other thermo-physical properties have been assumed to be the same as

those for n-dodecane. The latent heat and saturation pressure for each quasi-component have been assumed to be relatively weak functions of n .

This model has been applied to the analysis of heating and evaporation of droplets with initial radius 25 μm , initial temperature 300 K and constant velocity 1 m/s. The gas temperature and pressure have been assumed to be constant and equal to 880 K and 3 MPa respectively. The evaporation time predicted by the ETC/ED models using 20 quasi-components has been shown to be longer than in the case of 1 quasi-component. This can be attributed to the fact that at the final stages of droplet evaporation the heaviest species (large number of carbon atoms) become the dominant. They evaporate more slowly than more volatile species (small number of carbon atoms). Also they have higher wet bulb temperatures. There are also noticeable differences between the surface temperatures and radii predicted by the ETC/ED and ITC/ID models. Higher droplet surface temperatures, predicted by the ETC/ED model, compared with the ITC/ID model, are expected to affect the physical ignition delay of the autoignition of the fuel vapour [1].

MONO-COMPONENT DROPLETS: KINETIC MODELS

The limitation of the hydrodynamic models described above, even in the case of evaporation at high pressures, has been discussed in a number of papers, including [9-13]. In these papers the evaporation of n-dodecane (the nearest approximation to Diesel fuel) has been considered and a new model for the analysis of droplet heating and evaporation has been developed based on the combination of the kinetic and hydrodynamic approaches. In the immediate vicinity of droplet surfaces (up to about one hundred molecular mean free paths), the vapour and ambient gas dynamics have been studied based on the Boltzmann equation (kinetic region), while at larger distances the analysis has been based on the hydrodynamic equations (hydrodynamic region). Mass, momentum and energy fluxes have been conserved at the interface between these regions.

The predictions of this model have been shown to be as accurate as those of the model based on the kinetic equations in the whole domain, but both differed considerably (up to 10%) from the predictions of the hydrodynamic models for Diesel engine-like conditions. The practical application of this combined or kinetic modelling, however, requires the specification of some special boundary conditions at the droplet surface and at the interface between the kinetic and hydrodynamic regions. The kinetic boundary condition at the interface between vapour and its condensed phase has been presented as [10]:

$$f^{out} = \sigma f^e + (1 - \sigma) f^r \quad (v_x > 0), \quad (17)$$

where f^{out} is the overall distribution function of molecules leaving the interface from the liquid phase, σ is the evaporation coefficient, f^e is the distribution function of molecules in the saturated vapour at the liquid surface temperature, f^r is the distribution function of reflected molecules and v_x is the velocity component normal to the interface. In the equilibrium state the evaporation and condensation coefficients are equal. They will be referred to as the evaporation/condensation coefficient. In the above mentioned papers [9-13], it has been implicitly or explicitly assumed that the distribution function f^e is isotropic Maxwellian. The values of the evaporation/condensation coefficients have been assumed equal to 0.04 and 0.5 (the minimal and average value of this parameter of water) [9] or 1 [10-13]. None of these assumptions have been rigorously justified. The only practical way to perform this justification would be to base it on the molecular dynamic simulation at the interface region.

Most of the previous studies have applied the molecular dynamic approach to the analysis of the evaporation and condensation processing of monatomic or relatively simple polyatomic molecules, such as argon, water or methanol [14-18]. In our previous study [7], molecular dynamics simulations have been performed to study the evaporation and condensation of n-dodecane ($C_{12}H_{26}$) at liquid-vapour phase equilibria using the modified OPLS (Optimized Potential for Liquid Simulation) model. The interface thickness in equilibrium state has been predicted to be 1.2-2.0 nm. It has been shown that the molecular chains lie preferentially parallel to the interface in the liquid-vapour transition region. The predicted evaporation/condensation coefficient decreased from about 0.9 to about 0.3 when temperature increased from 400 K to 600 K. Typical molecular behaviours in the evaporation and condensation processes have also been presented and discussed.

Although this result still needs to be confirmed based on simulations including much larger numbers of molecules, it opens the way for a much more rigorous approach to the kinetic modelling of droplet heating and evaporation compared with the approaches used so far.

CONCLUSIONS

New solutions to the heat conduction equation, describing transient heating of an evaporating droplet, are described following [2]. These solutions take into account the effect of the reduction of the droplet radius due to evaporation, assuming that this radius is a linear function of time. The latter assumption does not allow us to

apply these solutions to describe the whole process, from the start of evaporation, until the moment in time when the droplet completely evaporates. However, these solutions are expected to be used to describe droplet heating and evaporation over a small time step when other parameters, except droplet radius and temperature, can be assumed constant. In this case they can be considered as generalisations of the approach currently used in all research and commercial computational fluid dynamics (CFD) codes known to us, in which it is assumed that droplet radius is constant during the time step.

New solutions to the heat conduction equation described in [3] are summarised, involving transient heating of an evaporating droplet and assuming that the time evolution of its radius $R_d(t)$ is known. Since $R_d(t)$ depends on the time evolution of the droplet temperature, an iterative process is required. The results of the calculations of droplet surface temperature, using this approach, are compared with the results obtained using the approach when the droplet radius is assumed to be a linear function of time during individual time steps for typical Diesel engine-like conditions. For sufficiently small time steps the time evolutions of droplet surface temperatures and radii predicted by both approaches coincide. Similarly to the case when droplet radius is assumed to be a linear function of time during the time step, the new solution predicts lower droplet temperatures and slower evaporation when the effects of the reduction of $R_d(t)$ are taken into account.

A simplified model for multi-component droplet heating and evaporation is discussed. Apart from the finite thermal conductivity of droplets and recirculation inside them, this model takes into account species diffusion inside droplets, based on the analytical solution to the species diffusion equation. The model has been implemented into a stand-alone zero-dimensional code and validated against the observed droplet temperatures in a monodisperse spray for various ethanol/acetone droplet mixtures. This simplified model has been generalised to take into account the effect of coupling between the droplets and the surrounding gas. A new approach to modelling multi-component droplets, including large numbers of components, heating and evaporation is discussed. This new approach is based on the replacement of a large number of actual components with a small number of quasi-components. It takes into account the effect of finite thermal and mass diffusion inside the droplet using the ETC/ED and ITC/ID models.

Two new solutions to the equation, describing the diffusion of species during multi-component droplet evaporation, are described. The first solution is the explicit analytical solution to this equation, while the second one reduces the solution of the differential transient species 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, assuming that this radius is a linear function of time. These solutions can be considered as the generalisations of the solutions reported earlier.

The evaporation and condensation of n-dodecane ($C_{12}H_{26}$), the closest approximation to Diesel fuel, have been investigated using the molecular dynamics (MD) simulation technique. Some preliminary results of this investigation are presented. The thickness of the transition layer between liquid and vapour phases at equilibrium is estimated to be 1.2-2.0 nm. It has been pointed out that the molecules at the liquid surface need to gain relatively large translational energy to evaporate. Vapour molecules with high translational energy can easily penetrate deep into the transition layer and condense in the liquid phase. The values of the evaporation/condensation coefficient at various liquid phase temperatures have been estimated.

ACKNOWLEDGMENT

The authors are grateful to the European Regional Development Fund Franco-British INTERREG IVA (Project C5, Reference 4005), EPSRC (grant EP/H001603/1), the Royal Society (UK) (Project JP090548) and RFBR Russia (grant 10-08-92602-KO_a) for the financial support of this project.

NOMENCLATURE

Symbol	Quantity	SI Unit
c	specific heat capacity	$J \cdot kg^{-1} \cdot K^{-1}$
C_m	constant introduced by Equation (15)	
D	diffusion coefficient	$m^2 \cdot s^{-1}$
f_m	distribution function	
h	heat transfer coefficient	$W \cdot m^{-2} \cdot K^{-1}$
h_0	parameter introduced in Equation (6)	
h_{0Y}	parameter introduced in Equation (11)	
k	thermal conductivity	$W \cdot m^{-1} \cdot K^{-1}$
L	latent heat of evaporation	$J \cdot kg^{-1}$
m	mass	kg
M	molar mass	$kg \cdot kmole^{-1}$
n	number of carbon atoms	
N_f	number of quasi-components	
Nu	Nusselt number	
Pe	Peclet number	
p_n	parameter introduced in Equation (5)	
q_{in}	parameter introduced in	

	Equation (11)	
q_n	parameter introduced in Equation (5)	
Q_n	parameter introduced in Equation (11)	
R	distance from the droplet centre	m
R_d	droplet radius	m
Sh	Sherwood number	
t	time	s
T	temperature	K
V_n	eigen function	
X	molar fraction	
Y	mass fraction	
α	parameter introduced by Equation (10) or constant introduced in Equation (14)	
β	constant introduced in Equation (14)	
γ	activity coefficient or constant introduced in Equation (14)	
ε_i	species evaporation rate	
κ	diffusivity	$m^2 \cdot s^{-1}$
κ_0	parameter introduced in Equation (5)	
λ	eigenvalues	
μ	dynamic viscosity	Pa.s
$\mu_0(t)$	parameter introduced in Equation (5)	
ρ	density	$kg \cdot m^{-3}$

Subscripts

b	boiling
d	droplet
eff	effective
f	final
g	gas
i	species
l	liquid
p	constant pressure
s	surface
v	vapour
0	initial

REFERENCES

- [1] S.S. Sazhin, Advanced models of fuel droplet heating and evaporation, *Progress in Energy and Combustion Science*, vol. 32, pp. 162-214, 2006.
- [2] S.S. Sazhin, P.A. Krutitskii, I.G. Gusev, M.R. Heikal, Transient heating of an evaporating droplet, *Int J Heat and Mass Transfer*, vol. 53, pp. 2826-2836, 2010.
- [3] S.S. Sazhin, P.A. Krutitskii, I.G. Gusev, M.R. Heikal, Transient heating of an evaporating droplet with presumed time evolution of its

- radius, *Int. J of Heat and Mass Transfer*, vol. 54(5-6), pp. 1278-1288, 2011.
- [4] S.S. Sazhin, A. Elwardany, P.A. Krutitskii, G. Castanet, F. Lemoine, E.M. Sazhina, M.R. Heikal, A simplified model for bi-component droplet heating and evaporation, *Int. J of Heat and Mass Transfer*, vol. 53(21-22), pp. 4495-4505, 2010.
- [5] S.S. Sazhin, A. Elwardany, P.A. Krutitskii, V. Depredurand, G. Castanet, F. Lemoine, E.M. Sazhina, M.R. Heikal, Multi-component droplet heating and evaporation: numerical simulation versus experimental data, *Int. J of Thermal Science*, vol. 50, pp. 1164-1180, 2011.
- [6] S.S. Sazhin, A. Elwardany, E.M. Sazhina, M.R. Heikal, A quasi-discrete model for heating and evaporation of complex multicomponent hydrocarbon fuel droplets, *Int. J of Heat and Mass Transfer*, vol. 54, pp. 4325-4332, 2011 .
- [7] B.Y. Cao, J.-F. Xie, S.S. Sazhin, Molecular dynamics study on evaporation and condensation of n-dodecane at liquid-vapour phase equilibria, *J Chemical Physics*, vol. 134, 164309 2011.
- [8] S.L. Mitchell, M. Vynnycky, I.G. Gusev, S.S. Sazhin, An accurate numerical solution for the transient heating of an evaporating spherical droplet, *Applied Mathematics and Computation*, vol. 217, pp. 9219-9233, 2011.
- [9] A.P. Kryukov, V.Y. Levashov, S.S. Sazhin, Evaporation of diesel fuel droplets: kinetic versus hydrodynamic models, *Int. J. Heat Mass Transfer*, vol. 47, pp. 2541-2549, 2004.
- [10] I.N. Shishkova, S.S. Sazhin, A numerical algorithm of kinetic modelling of evaporation processes, *J. Comput. Phys.*, vol. 218, pp. 635-653, 2006.
- [11] S.S. Sazhin, I.N. Shishkova, A.P. Kryukov, V.Yu. Levashov, M.R. Heikal, Evaporation of droplets into a background gas: kinetic modelling, *Int. J. Heat Mass Transfer*, vol. 50, pp. 2675-2691, 2007
- [12] S.S. Sazhin, I.N. Shishkova, A kinetic algorithm for modelling the droplet evaporation process in the presence of heat flux and background gas, *Atomization Sprays*, vol. 19, pp. 473-489, 2009.
- [13] S.S. Sazhin, I.N. Shishkova, M. Heikal, Kinetic modelling of fuel droplet heating and evaporation: calculations and approximations, *International J. of Engineering System Modelling and Simulation*, vol. 2, pp. 169-176, 2010.
- [14] T. Tsuruta, H. Tanaka, T. Masuoka, Condensation/evaporation coefficient and velocity distributions at liquid-vapour interface, *Int. J. Mass Heat Transfer*, vol. 42, pp. 4107-4116, 1999.
- [15] G. Nagayama, T. Tsuruta, A general expression for the condensation coefficient based on transition state theory and molecular dynamics simulation, *J. Chem. Phys.*, vol. 118, pp. 1392-1399, 2003.
- [16] T. Tsuruta, G. Nagayama, Molecular dynamics studies on the condensation coefficient of water, *J. Phys. Chem. B*, vol. 108, pp. 1736-1743, 2004.
- [17] T. Ishiyama, T. Yano, S. Fujikawa, Molecular dynamics study of kinetic boundary conditions at an interface between argon and its condensed phase, *Phys. Fluids*, vol. 16, pp. 2899-2906, 2004.
- [18] T. Ishiyama, T. Yano, S. Fujikawa, Molecular dynamics study of kinetic boundary conditions at an interface between a polyatomic vapor and its condensed phase, *Phys. Fluids*, vol. 16, pp. 4713-4726, 2004.