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New Models for Droplet Heating and Evaporation

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ABSTRACT

A brief summary of new models for droplet heating and evaporation, developed mainly at the Sir Harry Ricardo Laboratory of the University of Brighton during 2011-2012, is presented. These are hydrodynamic models for mono-component droplet heating and evaporation, taking into account the effects of the moving boundary due to evaporation, hydrodynamic models of multi-component droplet heating and evaporation, taking and not taking into account the effects of the moving boundary, new kinetic models of mono-component droplet heating and evaporation, and a model for mono-component droplet evaporation, based on molecular dynamics simulation. The results, predicted by the new models are compared with experimental data and the predictions of the previously developed models where possible.

Key words: Droplets, heating, evaporation, kinetic effects, molecular dynamics simulation

INTRODUCTION

The importance of accurate and CPU efficient modelling of droplet heating and evaporation in various engineering applications is widely recognised (Rahman *et al*., 2009; Leu and Huang, 2008; Faghri and Zhang, 2006; Heywood, 1988). Several reviews of various approaches to this modelling have been published (Sazhin, 2006). In typical engineering applications, this modelling is expected to take into account a number of processes, including the dynamics and break-up of droplets and possible autoignition of the vapour/air mixture, in the case of fuel droplets, in realistic three dimensional enclosures (Flynn *et al*., 1999). When modelling these individual processes, it is essential to find a compromise between the accuracy of the models and their CPU efficiency. In practice, this led to modelling based on over-simplistic sub-models of these processes (Sazhina *et al*., 2000). In most cases, these simplifications are at present unavoidable. In some cases, however, there seems to be room for considerable increase in the accuracy of the models without substantial CPU penalty.

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 (Sazhin, 2006). In a number of our earlier papers, some of which are discussed by Sazhin (2006, 2011), the range of applicability of some of these assumptions was investigated. The aim of this paper is to summarise some of the most recent developments in the modelling of droplet heating and evaporation processes, published mainly in 2010- 2012, 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 (Sazhin *et al.*, 2010a, 2011a). For multi-component droplets, including relatively small numbers of components, the new models are based on the analytical solution to the species diffusion equation inside the droplet ignoring the effects of the moving boundary (Sazhin *et al.*, 2010b, 2011b) and taking these effects into account (Elwardany *et al.*, 2011; Gusev *et al.*, 2012). The model designed to take into account large numbers of components is based on the introduction of the concept of quasi-components (Sazhin *et al.*, 2011c; Elwardany and Sazhin, 2012). A simplified kinetic model for droplet heating and evaporation is based on consideration of the kinetic effects as perturbations to the predictions of the hydrodynamic model (Sazhin *et al.*, 2010c). A new approach to calculating the evaporation coefficient of n-dodecane, the closest approximation to Diesel fuel, is described by Cao *et al.* (2011) and Xie *et al.* (2011, 2012). This coefficient is essential for the accurate kinetic modelling of droplet evaporation.

HYDRODYNAMIC MODELS

Assuming that droplet heating is spherically symmetric, the transient heat conduction equation inside droplets can be written as (Sazhin, 2006):

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

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:

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

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

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} (Sazhin, 2006):

$$T_{eff} = T_g + \rho_l L \frac{dR_d}{dt}/h \tag{4}$$

where, L is the latent heat of evaporation and 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 = const, the solution to the transient heat conduction Eq. 1, taking into account the reduction of droplet radius due to evaporation $R_d = R_{d0}(1-\alpha t)$ and the corresponding boundary (2) and initial (3) conditions, can be presented as (Sazhin *et al*., 2010a):

$$T(R) = \frac{1}{R\sqrt{R_d(t)}} \exp\left[-\frac{\alpha R_{d0} R^2}{4\kappa R_d(t)}\right] \times \left[\sum_{n=1}^{\infty} \Theta_n(t) \sin\left(\lambda_n \frac{R}{R_d(t)}\right) + \frac{\mu_0(t)}{1+h_0} \quad \frac{R}{R_d(t)}\right] \tag{5}$$

where:

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

$$\mu_0(t) = \overset{\circ}{\mu}(t)\sqrt{R_d(t)} \exp\left[\frac{R_d'(t) R_d(t)}{4\kappa}\right], \quad \overset{\circ}{\mu}(t) = M(t) R_d^2(t), \quad M(t) = \frac{h}{k_l} T_g + \frac{\rho_l}{k_l} L R_d'(t),$$

$$f_n = -\frac{\sin\lambda_n}{\| v_n \|^2 \lambda_n^2}, \quad v_n = \sin(\lambda_n \frac{R}{R_d(t)}) \qquad (n = 1,2,3,....), \quad \| v_n \|^2 = \frac{1}{2}\left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right)$$

$$h_0 = \frac{h(t)}{k_l} R_d(t) - 1 - \frac{R_d'(t) R_d(t)}{4\kappa} \text{ is constant}, \quad q_n = \frac{1}{\| v_n \|^2} \int_0^1 W_0(\xi) v_n(\xi) d\xi$$

λ_n are positive solutions to the equation:

$$\lambda \cos\lambda + h_0 \sin\lambda \tag{6}$$

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

$$W_0(\xi) = W_0(\frac{R}{R_d(t)}) = R_{d0}^{3/2} \xi T_0(\xi R_{d0}) \exp\left[\frac{R_d'(t) R_d(t)}{4\kappa} \xi^2\right]$$

$$\alpha = -\frac{k_g Sh}{2\rho_l c_{pg} R_d^2} \tag{7}$$

Solution 5 in combination with the equation for droplet radius:

$$\frac{dR_d}{dt} = -\frac{k_g Sh}{2\rho_l c_{pg} R_d} \tag{8}$$

can be applied for practical calculations only if the values for Nusselt and Sherwood numbers (Nu and Sh) are specified (Sazhin *et al*., 2010a). Solution 5 reduces to the one reported earlier by Sazhin (2006) in the limit when $\alpha = 0$.

In the general case of a time dependent h_0 the solution to Eq. 1 is reduced to the solution to the Volterra integral equation of the second kind (Sazhin *et al.*, 2010a).

Solution 5 was generalised to the case when droplet radius was assumed to be an arbitrary function $R_d(t)$ (Sazhin *et al.*, 2011a). 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 predictions of the model developed by Sazhin *et al.* (2011a) were shown to be in agreement with the predictions of the model based on Eq. 5 and the results reported by Mitchell *et al.* (2011). In the latter paper, the analysis was based on the direct numerical solution of Eq. 1, taking into account the effect of the moving boundary.

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 ($Y_{li}= Y_{li}(t, R)$) inside the droplets (Sazhin *et al.*, 2010b, 2011b):

$$\frac{\partial Y_{li}}{\partial t} = D_l \frac{\partial}{\partial R}\left(R^2 \frac{\partial Y_{li}}{\partial R}\right) \tag{9}$$

where, i>1, D_l is the liquid mass diffusivity. Equation 9 is solved subject to the boundary condition:

$$\alpha(\varepsilon_i - Y_{li}) = -D_l\left(\frac{\partial Y_{li}}{\partial R}\right)_{R=R_d-0}$$

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, $\varepsilon_i = Y_{vis}/\Sigma_i Y_{vis}$ 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 Eq. 7 of Gusev *et al.* (2012). 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 to Eq. 9 subject to the above mentioned boundary and initial conditions (Sazhin *et al.*, 2010b, 2011b):

$$\begin{aligned} Y_{li}(t,R) = \varepsilon_i + \frac{1}{R}\left(\left[\exp\left[D_l\left(\frac{\lambda_0}{R_d}\right)^2 t\right]\left(q_{i0} - \varepsilon_i(0)Q_0\right) - Q_0\int_0^t \frac{d\varepsilon_i(\tau)}{d\tau}\exp\left[D_l\left(\frac{\lambda_0}{R_d}\right)^2 (t-\tau)\right]d\tau\right]\sinh\left(\lambda_0\frac{R}{R_d}\right) + \right. \\ \left. \Sigma_{n=1}^{\infty}\left[\exp\left[-D_l\left(\frac{\lambda_n}{R_d}\right)^2 t\right]\left(q_{in} - \varepsilon_i(0)Q_n\right) - Q_n\int_0^t \frac{d\varepsilon_i(\tau)}{d\tau}\exp\left[-D_l\left(\frac{\lambda_n}{R_d}\right)^2 (t-\tau)\right]d\tau\right]\sin\left(\lambda_n\frac{R}{R_d}\right)\right) \end{aligned} \tag{10}$$

where, λ_0 is the non-zero solution to equation $\tanh \lambda = -\lambda/h_{0Y}$, λ_n (n>0) are the solutions to Eq. 6, with h_{0T} being replaced with h_{0Y}:

$$Q_0 = -\frac{1}{\|v_0\|^2}\left(\frac{R_d}{\lambda_0}\right)^2 (1+h_{oY})\sinh(\lambda_0)\; Q_n = \frac{1}{\|v_n\|^2}\left(\frac{R_d}{\lambda_n}\right)^2 (1+h_{oY})\sin(\lambda_n) \text{ when } n \geq 1$$

$$\|v_0\|^2 = -\frac{R_d}{2}\left(1+\frac{h_{0Y}}{h_{0Y}^2-\lambda_0^2}\right) \quad \|v_n\|^2 = \frac{R_d}{2}\left(1+\frac{h_{0Y}}{h_{0Y}^2-\lambda_n^2}\right) \text{ when } n \geq 1$$

$$q_{i0} = \frac{1}{\|v_0\|^2}\int_0^{R_d} R\, Y_{i0}(R)\sinh\left(\lambda_0\frac{R}{R_d}\right)dR,\; q_{in} = \frac{1}{\|v_n\|^2}\int_0^{R_d} R\, Y_{i0}(R)\sin\left(\lambda_n\frac{R}{R_d}\right)dR \text{ when } n \geq 1$$

$$h_{oY} = -\left(1+\frac{\alpha R_d}{D_l}\right)$$

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

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

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. 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 Eq. 10 (Gusev *et al*., 2012) and coupling with the ambient gas (Sazhin *et al*., 2011b) and has been tested against available experimental data (Sazhin *et al*., 2010b, 2011b).

The main limitation of the model, described above, 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 by Sazhin *et al*. (2011c) and further developed by Elwardany and Sazhin (2012) 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 was applied to Diesel fuel droplets which were approximated as a mixture of 21 actual components C_nH_{2n+2}, where, $n \geq 0$. These 21 actual components were replaced with up to 20 quasi-components (the maximal number of quasi-components in this model).

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

$$X_j = \int_{n_{j-1}}^{n_j} f_m(n)dn \tag{11}$$

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:

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

$M(n)=14n+2$ 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 $\gamma = 0$. $C_m(n_0, n_f)$ is the normalization constant.

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

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

The latent heat and saturation pressure for each quasi-component have been calculated by replacing n with $\bar{n}_f$. Other thermophysical properties have been assumed to be the same as those for n-dodecane in study of Sazhin *et al.* (2011c) or their dependence on n has been approximated by simple functions (Elwardany and Sazhin, 2012). 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 sec^{-1}. 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 (Sazhin, 2006).

It was pointed out that droplet surface temperatures and radii, predicted by a rigorous model taking into account the effect of all 20 quasi-components, are very close to those predicted by the model, using just five quasi-components (Sazhin *et al.*, 2011c). The importance of taking into account the dependence of density, viscosity, heat capacity and thermal conductivity of liquid components on carbon numbers and temperatures, has been demonstrated in (Elwardany and Sazhin, 2012).

KINETIC MODELS

The limitations of the hydrodynamic models described above, even in the case of evaporation at high pressures, have been discussed in a number of papers (Sazhin, 2006; Sazhin *et al.*, 2010c). 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.

Simple approximate formulae describing temporal evolution of Diesel fuel droplet radii and temperatures predicted by the kinetic model are suggested by Sazhin *et al.* (2010c). These formulae are valid in the range of gas temperatures relevant to Diesel engine-like conditions and fixed values of initial droplet radii, or in the range of initial droplet radii relevant to Diesel engine-like conditions and fixed values of gas temperature.

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:

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

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. 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 for water) or 1. 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.

MOLECULAR DYNAMICS MODELS

Most of the previous studies have applied the Molecular Dynamic (MD) approach to the analysis of the evaporation and condensation processes of monatomic or relatively simple polyatomic molecules, such as argon, water or methanol. In our earlier work Cao *et al.* (2011) molecular dynamics simulations have been performed to study the evaporation and condensation of n-dodecane ($C_{12}H_{26}$) at liquid-vapour phase equilibrium using the modified OPLS (Optimized Potential for Liquid Simulation) model. The predicted evaporation/condensation coefficient decreased from about 0.9 to about 0.3 when temperature increased from 400 to 600 K. Typical molecular behaviours in the evaporation and condensation processes were also presented and discussed.

A more detailed study of this problem, based on 720 molecules, was performed by Xie *et al.* (2011). In that study, the thickness of the transition layer between liquid and vapour phases at equilibrium was estimated to be 2.25-3.5 nm. It was pointed out that the molecules at the liquid surface need to have relatively large translational energy to evaporate. The vapour molecules with large translational energy can easily penetrate deeply into the transition layer and condense in the liquid phase. The values of the evaporation/condensation coefficient at various liquid phase temperatures were estimated. It was demonstrated that this coefficient decreases with temperature, in agreement with the prediction of the transition state theory. The molecular velocity distribution functions in the liquid phase and the interface were shown to be close to isotropic Maxwellian with temperatures equal to that of the liquid phase. These functions in the vapour phase, however, were shown to deviate from the classical isotropic Maxwellian distributions. They can be approximated as bi-Maxwellian, with temperatures in the direction normal to the interface larger than those in the directions parallel to the interface (Xie *et al.*, 2012).

Although, these results still need 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 mono-component droplet, are described following Sazhin *et al.* (2010a). 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, it is believed that these solutions could 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 by Sazhin *et al.* (2011a) are summarised. In these solutions it is assumed that the time evolution of a droplet's radius $R_d(t)$ is known. For sufficiently small time steps the time evolutions of droplet surface temperatures and radii predicted by both approaches coincide.

A simplified model for multi-component droplet heating and evaporation, suggested by Sazhin *et al.* (2010b, 2011b) 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. This simplified model was generalised to take into account the effect of coupling between the droplets and the surrounding gas (Sazhin *et al.*, 2011b) and the effect of the moving boundary on the species diffusion equation, as described by Gusev *et al.* (2012).

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 (Sazhin *et al.*, 2011c; Elwardany and Sazhin, 2012). It takes into account the effect of finite thermal and mass diffusion inside the droplet using the ETC/ED models.

Simple approximate formulae describing temporal evolution of Diesel fuel droplet radii and temperatures predicted by the kinetic model are briefly described, following Sazhin *et al.* (2010c).

The evaporation and condensation of n-dodecane ($C_{12}H_{26}$), the closest approximation to Diesel fuel, was investigated using the Molecular Dynamics (MD) simulation technique. The estimated values of the evaporation/condensation coefficient at various liquid phase temperatures are summarised.

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