*Sergei SAZHIN**
Sergey MARTYNOV
Tarsisius KRISTYADI
Cyril CRUA
Morgan HEIKAL
School of Engineering, Faculty of Science and Engineering,
University of Brighton, UK

Models for droplet heating and evaporation: application to simulation of the autoignition process in diesel engines

A review of liquid and gas phase models for fuel droplet heating and evaporation, suitable for implementation into CFD codes with a view to modelling the processes in Diesel engines, is presented. To describe properties of 'hot' Diesel fuel sprays, new sub-models for spray break-up, droplet heating and evaporation and Shell autoignition were implemented into the KIVA II CFD code. This customised version of the KIVA II code was used to simulate autoignition in Diesel engines. The results of simulation were shown to be consistent with in-house experimental data referring to autoignition timing at in-cylinder pressures from 5 to 9 MPa and an injection pressure of 160 MPa. The autoignition delay time is shown to be sensitive to the choice of liquid phase models for droplet heating, but not sensitive to the choice of gas phase models. It is recommended that the effective thermal conductivity liquid phase model and the gas phase model taking into account the effects of finite thickness of the thermal boundary layer are used for the simulation of the ignition process in Diesel engines. Some recent non-traditional developments of the models referring to droplet heating and evaporation are discussed. These are the model based on the coupled solution for the liquid and gas phases, the kinetic model of evaporation, and the dynamic decomposition technique for the solution of ordinary differential equations describing droplet heating and evaporation and the ignition of the fuel vapour/air mixture.
Key words: Diesel engines, autoignition, droplet heating, convection, radiation

INTRODUCTION

To simulate autoignition in a direct injection Diesel engine one needs to take into account a number of processes, including the dynamics and break-up of sprays, heating and evaporation of individual droplets and autoignition of the fuel vapour/air mixture in realistic three dimensional enclosures [1,2]. 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 [3,4]. For example, the detailed chemical mechanism of the autoignition process was replaced by reduced chemical models, one of the most popular of which seems to be the Shell model [5-10]. Droplet heating was typically modelled based on the assumption that the thermal conductivity of droplets is infinitely high [3,4]. In most cases, including the application of reduced chemical models, these simplifications are at present unavoidable. In some cases, however, there seems to be room for considerable increase in the accuracy of the spray autoignition model without substantial CPU penalty.

Bertoli and Migliaccio [11] were perhaps the first to draw attention to the fact that the accuracy of prediction, by computational fluid dynamics (CFD) code KIVA II, of the heating, evaporation and combustion of Diesel fuel sprays can be increased if the assumption of infinitely high thermal conductivity of liquid is relaxed. They suggested that the numerical solution of the heat conduction equation inside the droplets should be added to the solution of other equations in this code. Although this approach is expected to increase the accuracy of CFD predictions, the additional computational cost might be too

high for practical applications. A number of simplified models of droplet heating and evaporation, taking into account the effects of temperature gradient inside droplets and recirculation within them, have been suggested [12-20]. Some of these models were implemented into numerical codes focused on simulating droplet convective and radiative heating, evaporation and the ignition of a fuel vapour/air mixture [18-20]. In these papers, the results of implementation of the analytical solutions of the heat conduction equation inside the droplets, for constant convection heat transfer coefficient h, into a zero-dimensional numerical code, were reported. This code was then applied to the numerical modelling of fuel droplet heating and evaporation

in conditions relevant to Diesel engines [19]. It took into account the coupling between the liquid and gas phases and described the autoignition process based on the the above mentioned Shell model. The effect of the temperature gradient inside droplets was investigated by comparing the 'effective thermal conductivity' (ETC) model (see [15]) and the 'infinite thermal conductivity' (ITC) model, both of which were implemented into the zero-dimensional code. The approach based on the analytical solution of the heat transfer equation inside droplets was shown to be more CPU effective and accurate than that based on the numerical solution of the discretised heat conduction equation inside the droplet [18], and more accurate than the solution based on the parabolic temperature profile model [18]. The relatively small contribution of thermal radiation to droplet heating and evaporation allowed the authors to take it into account using a simplified model, which does not consider the variation in radiation absorption inside droplets [21-23] (a more

detailed analysis of thermal radiation absorption is discussed in [24-26]). It was pointed out that in the absence of break-up, the influence of the temperature gradient inside droplets on droplet evaporation under realistic Diesel engine conditions was generally small (less than about 5%). In the presence of the break-up process, however, the temperature gradient inside the droplets led to a significant decrease in evaporation time. It was recommended that the effect of the temperature gradient inside the droplets should be taken into account in computational fluid dynamics codes describing droplet break-up, heating and evaporation processes, and the ignition of the evaporated fuel/air mixture.

In this paper, the recently developed models of droplet heating and evaporation are reviewed. Then the results of implementation of these models into the KIVA II CFD code are discussed. The results of simulations of the autoignition process in an environment typical for Diesel engines, using the customised version of this code, are discussed and compared with in-house experimental data. Finally, some recent non-traditional approaches to modelling these processes are briefly summarised.

LIQUID PHASE MODELS

The liquid phase models actually used in CFD codes and the ones which can potentially be used are ITC (infinite thermal conductivity) and ETC (effective thermal conductivity) models. The ITC models are based on the energy balance equation of the droplet as a whole. The solution to this equation can be presented as [20]:

$$T = T_s = T_g + (T_{s0} - T_g)\exp\left(-\frac{3ht}{c_l \rho_l R_d}\right), \tag{1}$$

where T_{s0} and T_g are the initial droplet temperature and ambient gas temperature respectively, c_l and ρ_l are liquid specific heat capacity and density respectively. Droplet temperature T does not depend on the distance from the droplet centre R in this case.

Assuming that the process is spherically symmetric, the droplet transient heating in finite liquid thermal conductivity models is described by the following equation [14]:

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

where $K_l = k_l/(c_l\,\rho_l)$ is the liquid thermal diffusivity, k_l is the liquid thermal conductivity, assumed to be constant, T is specified at the initial moment of time as $T|_{t=0}=T_0(R)$, P takes into account the radiative heating of a droplet. The boundary condition at $R=0$ follows from the problem symmetry $\partial T/\partial R|_{R=0} = 0$. Assuming that the droplet is heated by convection from the surrounding gas, and cooled due to evaporation, the boundary condition at the droplet surface can be written as:

$$h(T_g - T_s) = -\rho_l L\frac{dR_d}{dt} + k_l \frac{\partial T}{\partial R}|_{R=R_d},$$

where L is the latent heat of evaporation, h is the convection heat transfer coefficient describing heat obtained by droplets from gas (due to heating of fuel vapour this heat is less than the heat lost by gas). Effects of swelling are ignored at this stage.

The general analytical solution of Equation (2), taking into account the changes in droplet radius due to evaporation, would be a difficult task. This could be considerably simplified if we take into account that this solution is used in the numerical analysis when the time step is small. In this case we can assume that the droplet radius is constant, but the effect of evaporation can be taken into account by replacing T_g with the effective temperature [7]:

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

The solution to Equation (2) for h=const can be presented as [14]:

$$T = T_{eff} + \frac{R_d}{R}\sum_{n=1}^{\infty}\left\{\left[q_n - \frac{\sin\lambda_n\ \mu_0(0)}{\lambda_n^2 \parallel V_n \parallel^2}\right]\exp(-\kappa_0\lambda_n^2\ t)\right.$$

$$\left. - \frac{\sin\lambda_n}{\lambda_n^2 \parallel V_n \parallel^2}\int_0^1 \frac{d\mu_0(\tau)}{d\tau}\exp\left[-\kappa_0\lambda_n^2(t-\tau)\right]d\tau\right\}\sin\left(\frac{\lambda_n R}{R_d}\right) + \frac{R_d}{R}\sum_{n=1}^{\infty}\ \frac{p_n}{\kappa_0\lambda_n^2}\left[\ 1-\exp(-\kappa_0\lambda_n^2 t)\right]\sin\left(\frac{\lambda_n R}{R_d}\right) \tag{3}$$

where

$\mu_0 = \frac{hT_{eff}(t)R_d}{k_l}$, $q_n = \frac{1}{\| V_n \|^2}\int_0^1 \overline{T} V_n(R) d(R/R_d)$, T_{d0} is the droplet initial temperature distribution, $\overline{T} = RT_{d0}(R)/R_d$, $\kappa_0 = k_l/(c_l\rho_l R_d^2)$, λ_n are solutions to the equation:

$\lambda_n \cos\lambda_n + h_0 \sin\lambda_n = 0$, $h_0 = \frac{hr_d}{k_l} - 1$, $\| V_n \|^2 = 0.5(1 - \sin 2\lambda_n / 2\lambda_n)$, $V_n = \sin(\lambda_n R/R_d)$,

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

If we take into account the distribution of absorption of thermal radiation inside droplets, using the simplified model suggested in [24], we can present this term as:

$$P(R) = \frac{3\pi}{R_d c_l \rho_l}\int_{\lambda_1}^{\lambda_2} w(\bar{r},\lambda) Q_a B_\lambda(T_{ext}) d\lambda, \tag{4}$$

where $\bar{r} = R/R_d$, $B_\lambda(T_{ext})$ is the Planck function:

$$B_\lambda(T_{ext}) = \frac{C_1}{\pi\lambda^5\left[\exp\left(C_2/(\lambda T_{ext})\right) - 1\right]},$$

C_1= 3.742 10^8 W μm^4/m^2, C_2 = 1.439 x10^4 μm K. λ is the wavelength in μm. It was assumed that the external thermal radiation is that of a black body. $w(\bar{r},\lambda)$ is the normalised spectral power of radiation per unit volume absorbed inside the droplet. Using the MDP_0 approximation (see [24]) and a number of additional assumptions and simplifications, the following expressions were obtained [24]:

$$w = \frac{\left[1 - \mu_* \Theta(\bar{r} - (1/n))\right]\left(\bar{r}^2 + \bar{\gamma}\right)}{\left[0.6(1-\mu_c^5) - \mu_c^3/n^2\right] + \bar{\gamma}(1-\mu_c^3)} \tag{5}$$

where $\bar{\gamma} = (1.5/\tau_0^2) - (0.6/n^2)$, $\mu_* = \sqrt{1 - \left(\frac{1}{n\bar{r}}\right)^2}$, $\mu_c = \sqrt{1 - \left(\frac{1}{n}\right)^2}$, $\tau_0 = a_\lambda R_d = 4\pi\kappa_\lambda R_d/\lambda$,

$\Theta(x) = 0$ when $x < 0$, and $\Theta(x) = 1$ when $x \geq 0$; or

$$w = \frac{\xi^2\tau_0^3}{3}\frac{\exp\left[-\xi(\tau_0 - \tau)\right]}{\tau_0(\xi\tau_0 - 2) + (2/\xi)\left[1 - \exp(-\xi\tau_0)\right]}, \tag{6}$$

where $\tau = a_\lambda R$, $\xi = 2/(1+\mu_c)$. Equation (5) was used when $\tau_0 < n\sqrt{2.5}$, otherwise Equation (6) was used. As in Equation (4) λ_1 and λ_2 describe the spectral range of thermal radiation which contributes to droplet heating. It was assumed that λ_1=0.5 μm, λ_2=6 μm, and n was calculated as [27]:

$$n = n_0 + 0.02\frac{\lambda - \lambda_m}{(\lambda - \lambda_m)^2 + 0.001}, \tag{7}$$

where n_0=1.46, λ_m=3.4 μm. This model was generalised in [25] to the case of asymmetric illumination of droplets. Further refinements of this model were reported in [26].

Ignoring the dependence of the distribution of thermal radiation absorption on R and t, we can present the expression for $P(R)$ as [21-23]:

$$P(R) = \frac{3\sigma}{\rho_l c_l} a R_d^{b-1} T_{ext}^4, \tag{8}$$

where we assumed that the radiation temperature θ_R is equal to the external temperature $T_{ext.}$ For low sulphur ESSO AF 1313 diesel fuel, it was found that the best approximation for a and b in the ranges $5 \le R_d \le 50\,\mu$m and $1000 \le T_{ext} \le 3000$ K is provided by the functions [22]:

$$a = 0.10400 - 0.05432\,(T_{ext}/1000) + 0.00800\,(T_{ext}/1000)^2,$$

$$b = 0.49162 - 0.09837\,(T_{ext}/1000) - 0.007857\,(T_{ext}/1000)^2.$$

The generalisation of the above model to the case of moving droplets (ETC model) can be achieved by replacing the thermal conductivity of liquid k_l by the effective thermal conductivity $k_{eff} = \chi\, k_l$, where the coefficient χ varies from about 1 (at droplet Peclet number <10) to 2.72 (at droplet Peclet number >500) [15]. The variations of all parameters with temperature and time were accounted for when analytical solution (3) was incorporated into a numerical code [14,18,19].

The model suggested in [12] is based on an *a priori* assumption about the temperature profile inside the droplet in the form:

$$T(r,t) = T_c(t) + [T_s(t) - T_c(t)](R/R_d)^2, \tag{9}$$

where $T_c(t)$ and $T_s(t)$ are the temperatures in the centre ($R=0$) and on the surface ($R=R_d$) of the droplet respectively. The boundary condition at $R=0$ is satisfied. Substitution of Equation (9) into the boundary condition at $R=R_d$ gives [12]:

$$T_s - T_c = \zeta(T_g - T_s)/2 + \rho_l L r_d \frac{dR_d}{dt}/(2k_l), \tag{10}$$

where $\zeta = 0.5\,\mathrm{Nu}\, k_g / k_l$, $\mathrm{Nu} = 2\,h\,R_d/k_g$ is the Nusselt number. Equation (6) should satisfy the equation of thermal balance, which is obtained from integration of Equation (2) along the radius [12]:

$$\frac{\rho_l c_l R_d}{3}\frac{d\bar{T}}{dt} = h(T_g - T_s) + \rho_l \frac{dR_d}{dt}[L - c_l(T_s - \bar{T})], \tag{11}$$

where

$$\bar{T} = \frac{3}{R_d^3}\int_0^{R_d} R^2 T(R)\,dR.$$

From the definition of $\frac{dR_d}{dt}$ and Eqs.(10) it follows [12]:

$$T_s = (\bar{T} + 0.2\zeta T_g)/\psi + 0.2\zeta\rho_l R_d \frac{dR_d}{dt} L/(k_l\psi), \tag{12}$$

where ψ= 1+0.2 ζ. Equations (10) and (12) give the full solution of the problem of droplet heating in the presence of evaporation. As shown in [12], in the absence of evaporation, this model gives reasonably accurate results unless the time is close to zero. In the same paper a correction to this model was suggested which gives accurate results over the whole time period starting with *t=0*. An additional version of this model, taking into account the effect of evaporation, is discussed in [13]. This model was based on the assumption that T_s = const. The *d*-squared law of droplet evaporation was modified to take into account droplet heating. The modified form of the *d*-squared law, called the elliptic law, was based on the elliptic presentation of the plot of droplet radius versus time.

The implementation of the parabolic model into the research version of the VECTIS code of Ricardo Consulting Engineers was based on Equation (9), where T_s is calculated from Equation (12) without evaporation terms [28]. The value of $\bar{T}$ in the latter equation is taken from the previous time step. The parabolic model modification of droplet heating was incorporated into the ODEs for droplet temperature and radius. As follows from VECTIS computations for realistic Diesel engine parameters, the parabolic model predicts the initial rate of increase of droplet surface temperature to be slightly less when compared with the prediction of the isothermal model. The above mentioned parabolic model is much simpler than the numerical solution of Equation (2) and the rigorous analytical solution of this equation (solution (3)).

The values of *h* are controlled by the conditions in the gas phase, discussed briefly in the next section. Various approximations for *h* are usually described in terms of the corresponding approximations for the Nusselt number $Nu = hR_d / k_g$. Droplet heating, described in the previous section, is accompanied by droplet evaporation, described by the following equation:

$$\frac{dR_d}{dt} = -\frac{k_g Sh}{2\rho_l c_{pg} R_d}, \tag{13}$$

where k_g is the gas thermal conductivity, c_{pg} is the gas specific heat capacity at constant pressure, Sh is the Sherwood number.

The numerical algorithm, based on the analytical solution of heat conduction equation (Equations (3) and (13)), and the simplified thermal radiation absorption model, was used to develop a zero-dimensional code [18,19]. This code took into account the temperature gradient inside the droplets, the coupling between liquid and gas phases and described the autoignition process based on the Shell model. It was used to study the effects of temperature gradient inside fuel droplets on droplet evaporation, break-up and the ignition of fuel vapour/air mixture. The predictions of the code were validated against experimental data published by Belardini et al [29], Nomura et al [30], and Tanabe et al [31]. In the absence of break-up, the influence of temperature gradient on droplet evaporation in realistic Diesel engine conditions was generally small (1-3%). In the presence of the break-up process, however, the temperature gradient inside droplets could lead to a significant decrease in the evaporation time under the same conditions. This was attributed to the fact that the temperature gradient inside droplets leads to a substantial increase in droplet surface temperature at the initial stages of heating. This increase, in turn, leads to a decrease in the droplet surface tension and threshold radii of the unstable droplets, assuming that bag and stripping break-ups are the dominant mechanisms of droplet break-up. Even in the absence of break-up, the effect of temperature gradient inside droplets led to a noticeable (up to about 20%) decrease of the total ignition delay time (comprising the physical and chemical ignition delays). In the presence of break-up, this effect was enhanced substantially, more than halving the total ignition delay. This reduction of the total ignition delay time is understood to be a combined effect of the influence of increased droplet surface temperature on the chemical ignition delay, and the influence of this temperature on droplet evaporation (in the presence of break-up processes). It was recommended that the effects of temperature gradient inside droplets are taken into account in computational fluid dynamics codes which describe droplet break-up and evaporation processes, and the ignition of the evaporated fuel/air mixture.

GAS PHASE MODELS

The difference between various gas models is essentially described in terms of different approximations of Nusselt and Sherwood numbers. These approximations are briefly summarised below [19].

Model 0:

$$Nu = 2\frac{\ln(1+B_M)}{B_M}\left(1+0.3\,\mathrm{Re}_d^{1/2}\,\mathrm{Pr}_d^{1/3}\right), \qquad Sh = 2\ln(1+B_M)\left(1+0.3\,\mathrm{Re}_d^{1/2}\,Sc_d^{1/3}\right),$$

where B_M is the Spalding mass number, Re_d, Pr_d, Sc_d are Reynolds (based on droplet diameter), Prandtl and Schmidt numbers respectively.

Model 1:

$$Nu = 2\frac{\ln(1+B_T)}{B_T}\left(1+0.3\,\mathrm{Re}_d^{1/2}\,\mathrm{Pr}_d^{1/3}\right), \qquad Sh = 2\ln(1+B_M)\left(1+0.3\,\mathrm{Re}_d^{1/2}\,Sc_d^{1/3}\right),$$

where B_T is the Spalding heat transfer number.

Model 2:

$$Nu = 2\frac{\ln(1+B_T)}{B_T}\left(1+0.3\,\mathrm{Re}_d^{1/2}\,\mathrm{Pr}_d^{1/3}/F(B_T)\right), \qquad Sh = 2\ln(1+B_M)\left(1+0.3\,\mathrm{Re}_d^{1/2}\,Sc_d^{1/3}/F(B_M)\right),$$

where

$$F(B_{T,M}) = (1+B_{T,M})^{0.7}\,\frac{\ln(1+B_{T,M})}{B_{T,M}}.$$

Model 3:

$$Nu = 2\frac{\ln(1+B_T)}{B_T}\left(1+\frac{1}{2}[(1+\mathrm{Re}_d\,\mathrm{Pr}_d)^{1/3}\ \max[1,\mathrm{Re}_d^{0.077}]-1]\right),$$

$$Sh = 2\frac{\ln(1+B_M)}{B_M}\left(1+\frac{1}{2}[(1+\mathrm{Re}_d\,Sc_d)^{1/3}\,\max[1,\mathrm{Re}_d^{0.077}]-1]\right).$$

Model 4:

$$Nu = 2\frac{\ln(1+B_T)}{B_T}\left(1+[(1+\mathrm{Re}_d\,\mathrm{Pr}_d)^{1/3}\,\max[1,\mathrm{Re}_d^{0.077}]-1]/[2F(B_T)]\right),$$

$$Sh = 2\frac{\ln(1+B_M)}{B_M}\left(1+[(1+\mathrm{Re}_d\,Sc_d)^{1/3}\,\max[1,\mathrm{Re}_d^{0.077}]-1]/[2F(B_B)]\right).$$

Model 5:

$$Nu = 2\frac{\ln(1+B_T)}{B_T}\left(1+0.276\,\mathrm{Re}_d^{1/2}\,\mathrm{Pr}_d^{1/3}/F(B_T)\right), \qquad Sh = 2\ln(1+B_M)\left(1+0.276\,\mathrm{Re}_d^{1/2}\,Sc_d^{1/3}/F(B_M)\right).$$

Model 6:

$$Nu = \frac{2+0.57\,\mathrm{Re}_d^{1/2}\,\mathrm{Pr}_d^{1/3}}{(1+B_F)^{0.7}}, \qquad Sh = 2\frac{1+0.435\,\mathrm{Re}_d^{1/2}\,Sc_d^{1/3}}{(1+B_M)^{0.7}},$$

where

$B_F = \dfrac{c_{pf}(T_g-T_s)}{L}\left(1-\dfrac{Q_L}{Q_c}\right)$, Q_c is the heat rate supplied to the droplet by convection, Q_L is the heat rate spent on droplet heating. Note that in the original definition of B_F, the effect of thermal radiation was incorporated.

Models 0-5 are based on the combination of fitting experimental data and theoretical analysis of the processes (semi-theoretical models). Model 6 is based on correlations which are inferred merely from the analysis of experimental data.

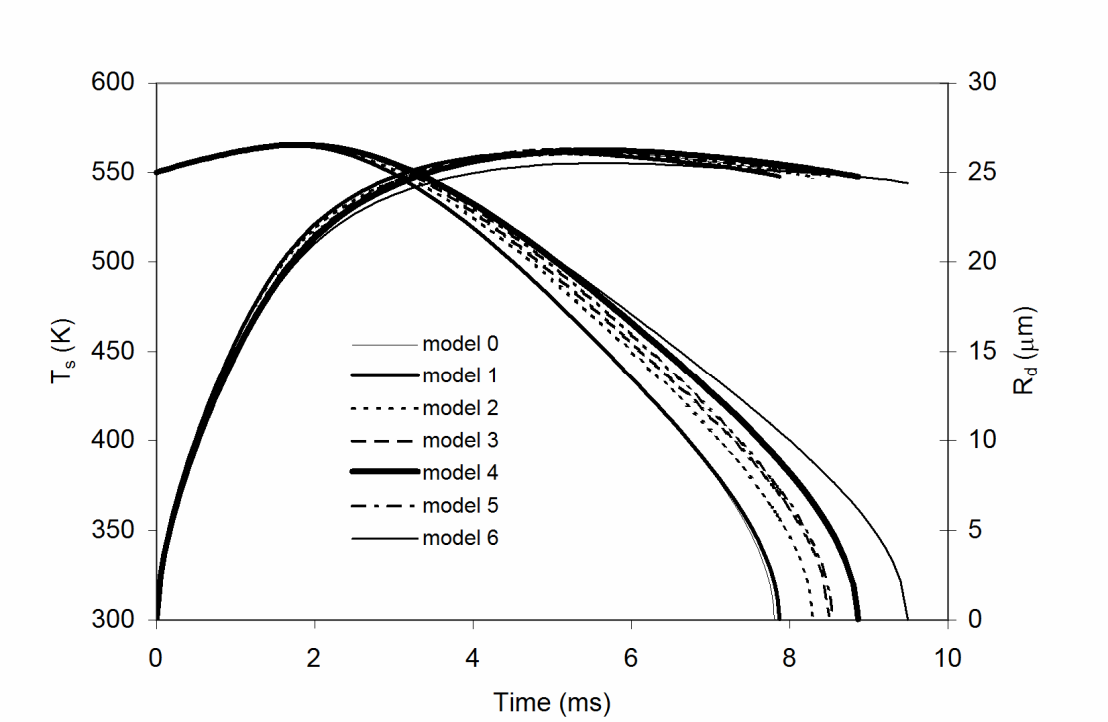

Fig. 1 Plots of T_s and R_d versus time for the initial gas temperature T_{g0} = 880 K, gas pressure p_{g0}=3 MPa, droplet temperature T_{d0} = 300 K, radius R_{d0}=25 μm and relative velocity v_{d0}=1 m/s. The overall volume of injected liquid fuel was taken equal to 1 mm^3, and the volume of air, where the fuel was injected, was taken equal to 883 mm^3, T_{ext} = 2000 K. The results were obtained based on the effective thermal conductivity (ETC) model, the analytical solution of the heat conduction equation, and using seven gas phase models.

The liquid and gas models described above were tested for the values of parameters typical for Diesel engines. All these models were implemented into the above mentioned zero dimensional in-house CFD code, taking into account coupling between gas and liquid phases. At first the liquid model was fixed and the effect of gas models on droplet heating and evaporation was investigated [19]. The break-up processes and chemical reactions in the gas phase were ignored at this stage. The temperature gradient inside droplets and recirculation within droplets were taken into account based on the ETC model. The physical properties of fuel (except radiation properties) were taken as for n-dodecane (see Appendix A in [19]). The radiation effect was described by Equation (8). Droplets were injected at room temperature (T_{d0}=300 K) into air at a temperature of 880 K and pressure of 3 MPa. The overall volume of injected liquid fuel was taken to be equal to 1 mm^3, and the volume of air, where the fuel was injected, was taken to be 883 mm^3. In this case, provided that all fuel is evaporated without combustion, the fuel vapour/air mixture is expected to become close to stoichiometric [19]. The radiation temperature was assumed equal to 2000 K. The initial droplet radius and relative velocity were assumed to be equal to 25 μm and 1 m/s, respectively. The plots of droplet radius R_d and surface temperature T_s versus time for gas phase Models 0-6 are shown in Fig. 1.

As follows from this figure, the effect of the choice of gas model on time evolution of T_s is relatively small, especially at the very initial stage of heating. However, the effect on time evolution of R_d is clearly visible. The difference in the evaporation times predicted by various models can reach almost 20%. If we assume that Model 6 is the most accurate, as the one based merely on experimental data, then we can conclude that the most accurate semi-theoretical model is Model 4 and the least accurate is Model 0, used in [18]. This is generally confirmed by the results of comparison for other values of parameters [19]. Our comparison of predictions of liquid phase models was based on Model 4 for the gas phase. The main advantage of Model 4 compared with Model 6 is that the former takes into account the underlying physics more accurately than the latter [19].

In contrast to the cases without thermal radiation, the maxima on the temperature plots can be seen. As pointed out in [32,33], in the absence of radiation, the droplet temperature approaches some equilibrium or ‘wet-bulb' temperature, at

which all of the heat coming to the droplet surface from the gas is spent on evaporation (latent heat), and the net heat penetrating to the liquid phase becomes zero. In the presence of radiation, however, the droplet surface temperature continues to rise above that wet-bulb temperature, due to radiation energy supplied to the droplet interior. As the droplet surface temperature rises, the heat coming to the droplet surface by convection decreases, but the heat spent in evaporation increases. As a result, the direction of the net heat flux inside the droplet becomes negative (heat flows from droplet centre to droplet surface). During the process of evaporation, the total radiative power absorbed by the droplet (droplet volume times *P(R)*) decreases approximately proportionally to $R_d^{2.6}$. The power lost by the droplets during the conduction heat transfer from the droplet centre to the droplet surface is approximately proportional to droplet surface area divided by droplet radius (proportional to R_d). Hence, at a certain droplet radius, the power lost by the droplet during the conduction heat transfer becomes equal to the radiative power absorbed by the droplet. This corresponds to the maximum droplet average temperature. The moment this happens is expected to be close to the moment when the maximum droplet surface temperature is reached.

Using the same input parameters as in Fig. 1, the plots of droplet radius R_d and surface temperature T_s versus time were calculated for gas phase Model 4 and ITC and ETC liquid phase models [19]. The evaporation time predicted by both liquid phase models turned out to be close. However, a noticeable difference in temperatures was observed at the initial stage of droplet heating and evaporation. This led to a rather strong dependence of the predicted total autoignition delay on the choice of liquid phase model. This is related to strong non-linear dependence of the chemical part of this delay on gas temperature in the vicinity of droplets. Also, the choice of a liquid phase model is important when droplet break-up processes are taken into account [18,19]. Several liquid and gas phase models were used for modelling droplet heating and evaporation, together with the autoignition of the mixture of air and fuel vapour produced by evaporating droplets [18,19]. The chemical part of the autoignition process was modelled based on the Shell model in the form suggested in [10]. It was pointed out that the total ignition delay (physical and chemical delays) depends weakly on the choice of the gas phase model. Its dependence on the choice of the liquid phase model turned out to be strong, in agreement with [18]. In the presence of droplet break-up processes, the evaporation time and the total ignition delay depend both on the choice of gas and liquid phase models [18,19].

The models described above for droplet heating and evaporation were implemented into a customised version of the KIVA-II computational fluid dynamics (CFD) code [34] alongside the Taylor-analogy break-up (TAB) model (the default model in KIVA-II) [35], and the conventional and modified version of the WAVE break-up model [36]. In the modified version of the WAVE model, the break-up rate constant is modified in order to take into account the damping effect of injection acceleration on the rate of spray break-up:

$$B_1 = B_1^{eq} + 3.8 \cdot \left(a^+\right)^{0.2}, \tag{14}$$

where $B_1^{eq} = 10$ is the break-up time of the conventional WAVE model [37], and a^+ is a dimensionless acceleration parameter. This empirical equation was suggested to describe better the highly transient initial stage of spray penetration. In all cases, the blob injection method was used [37]. In the Shell model, the pre-exponential constant for the reaction rate for the production of the branching agent was set to value $A_{f4} = 3 \cdot 10^6$ [3,10]. The results of calculations were compared with the results of in-house measurements of the ignition delay in Diesel sprays. The experimental setup used for these measurements is briefly described below.

EXPERIMENTAL SETUP

The spray rig facility is a rapid compression machine based around a single cylinder Ricardo Proteus test engine. An optical chamber, 80 mm in length and 50 mm in diameter, was fitted on to the cylinder head to enable the full length of the developed fuel spray to be viewed. This chamber provided a near quiescent high-pressure environment, with realistic in-cylinder conditions being achieved by conditioning of the intake air. The size and cylindrical shape of the chamber offered sufficient space for the fuel spray to develop without wall impingement. The flow field in the chamber was quiescent to avoid disturbances in the spray development due to airflow.

In order to record the autoignition process, two high-speed CCD video cameras recording 27,000 frames per second were placed at 90° to each other. Both cameras were triggered by the same dedicated signal emitted by the custom-built FIE controller. The resolution of the video recordings was 128×64 pixels × 256 grey levels, with a sensitivity equivalent to 3,000 ISO. In order to further maximise the sensitivity of the recordings, the lens was set to its widest aperture (f/1.9). The time at which the first fuel droplets were seen leaving the nozzle was measured to be 0.37 ms after the start of the recording for an injection pressure of 160 MPa. The data were adjusted to compensate for this delay. More information on the experimental setup can be found in [38].

The test cases chosen for the analysis were based on the measurements of sprays under realistic conditions of operation for a light-duty Diesel engine with a single-hole injector of 0.2 mm in diameter, located on the axis at the top centre of a cylindrical combustion chamber. The fuel injection pressure was 160 Mpa, the monitored in-cylinder pressures at TDC were 5, 6, 7.2 and 8.5 Mpa, and the in-cylinder temperature was calculated to be 800 K. The rate of injection was measured as a function of time using a Lucas rate tube. The ignition delay time was defined as the time from the start of injection to the first appearance of a visible flame on the video recordings.

RESULTS

The recorded measurements of Diesel spray autoignition were used to test the spray models mentioned earlier. This testing was focused on analysis of the sensitivity of predicted autoignition delay to the choice of ETC and ITC liquid phase models, gas phase models and spray break-up models. Simulations were performed for a constant-volume chamber of 40 mm in diameter and 100 mm in height, covered by a non-uniform two-dimensional axi-symmetric mesh of 20 x 48 grid points. The temperature of the injected fuel was assumed equal to 400 K. The properties of Diesel fuel were approximated by those of n-dodecane ($C_{12}H_{26}$). The total number of parcels introduced to the domain during the injection pulse was set to 1,000.

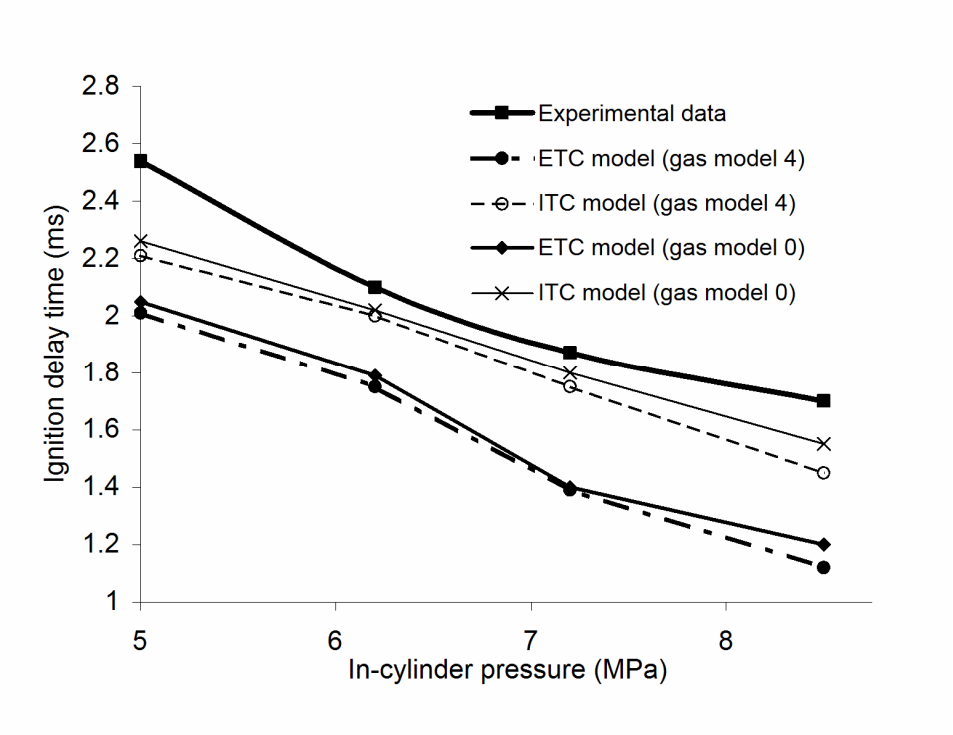

Figure 2. Predicted and experimentally measured ignition delay times versus in-cylinder pressure for ETC and ITC liquid-phase models and models 0 and 4 for the gas phase. 1,000 droplet parcels with initial droplet temperature 400 K were injected into a cylinder with initial temperature 800 K. The conventional WAVE spray break-up model was used.

Firstly the variation of the ignition delay time predicted using various spray break-up models, the ETC liquid heating model and gas-phase model 4 were investigated. It was shown that the predicted rate of decrease of the ignition delay with increasing in-cylinder pressure is in good agreement with the results of measurements. This relates to the fact that smaller droplets are formed at higher in-cylinder pressures when better atomisation of the spray is expected. Variations in the ignition delay times predicted using various models of spray break-up can be explained by the large contribution of the spray atomisation, evaporation and mixing processes to the total ignition delay time. Thus, the TAB model predicts faster spray atomisation and shorter ignition delays, in comparison with the conventional and modified WAVE models. The ignition delays for the modified and conventional WAVE models were shown to practically coincide. This can be explained by the fact that the transient stage of injection is short (~0.4 ms) compared with the ignition delay time (~2 ms), and therefore cannot lead to a significant autoignition delay. Note, the spray model is not expected to predict the exact coincidence between predicted and measured ignition delays due to a rather arbitrary choice of the parameter $A_{f4} = 3 \cdot 10^6$ in the Shell model.

Figure 2 shows the effect of the liquid-phase model (ETC and ITC) and the gas phase model (Models 0 and 4) on the ignition delay time. As follows from this figure, the choice of liquid phase model can significantly affect the predictions

of autoignition delay. At the same time, the effect of the choice of gas model is relatively small. Thus, at high in-cylinder pressures the difference between the ignition delays predicted using ETC and ITC models can be about 30%. In agreement with [18,19], the ignition delay predicted by the ETC model is always less than the one predicted by the ITC model. As already mentioned, the model is not expected to predict exact coincidence between predicted and measured ignition delays due to a rather arbitrary choice of the parameter A_{f4}.

NON-TRADITIONAL DEVELOPMENTS

The analysis presented so far is valid for quasi-stationary processes (the boundary layer around a droplet has enough time to develop). The general problem of heating a spherical body (droplet), based on the coupled heat conduction equations in the body and the gas was solved in [39,40]. Radiation was not taken into account, the initial temperature inside the body was assumed to be constant and the volume occupied by the gas was assumed to be infinitely large. A more realistic model describing the process of heating a spherical body (droplet) immersed in a hot gas was suggested and described in [41]. The droplet was assumed to be semi-transparent. The domain occupied by the gas was assumed to be spherical, finite and described by radius R_g. The outer boundary of this domain was kept at constant temperature. As in [39,40], the contribution of the flow around the droplet was ignored. The initial radial distribution of temperature in the droplet was taken into account. Newton's conventional law of body heating was generalised by introducing a correction for either the initial gas temperature or convective heat transfer coefficient. Explicit expressions for these corrections were obtained. The results were analysed for values of parameters relevant to the problem of stationary liquid fuel droplet heating in conditions similar to those in a Diesel engine. It was pointed out that for small Fo the correction of the convective heat transfer does not depend on the size of the domain, and reaches about 2.8 at Fo=0.1. For Fo>1, the correction becomes sensitive to the size of the domain. For large domains this correction was shown to be the same as can be deduced from the earlier model suggested in [39]. Ignoring these corrections (which is a universal practice in most engineering computational fluid dynamics (CFD) codes) is expected to lead to unacceptably large errors.

Also, we should note that most of the currently used 'hydrodynamic' models for droplet evaporation implicitly assume that the rate of detachment of molecules of fuel is such that the concentration of fuel vapour at the droplet surface is maintained at saturation level. The applicability of this assumption to the problem of modelling fuel droplet evaporation in realistic Diesel engines is not at first evident. In [42] a comparative analysis of hydrodynamic and kinetic approaches to the problem of Diesel fuel droplet evaporation was presented, based on an approximate kinetic model developed earlier. A more rigorous numerical analysis of the kinetic processes related to droplet evaporation is discussed in [43,44]. Although the importance of kinetic effects in Diesel engines have been clearly demonstrated in these papers, it remains unclear how these effects can be taken into account in CFD codes. Further investigation of these effects, leading to the development of a practical model, suitable for implementation into these codes, is required.

The solution of the system of ordinary differential equations (ODEs), describing droplet dynamics, heating and evaporation, and chemical reactions inside computational cells, is widely based on its decomposition. The simplest decomposition of this system is based on the sequential solution of the individual subsystems of which the system is comprised. In this approach, the solution of each individual subsystem, for a given subset of variables, is based on the assumption that all the other variables are fixed. The sequence of the solution of individual subsystems is often chosen rather arbitrarily and the results sometimes vary substantially depending on the order in which the subsystems are solved. In the case of a multi-scale system, the reliability of this approach becomes altogether questionable. One of the ways to overcome these problems is based on the idea that the multi-scale nature of ODEs needs to be investigated before any attempt to solve them is made. The development of a new, universal method of decomposition of the system of ODEs, allowing for changes in the nature of decomposition with time (dynamic decomposition), was the main objective of [45]. The formal approach to ODE system decomposition in that paper was based on the division of system variables into 'fast' and 'slow'. This in turn led to the division of the system onto 'fast' and 'slow' subsystems. Linearised variations of slow variables during the time evolution of the fast variables were taken into account as the first order approximation to the fast manifold. The usefulness of this division depends on whether the 'fast' subsystem has lower dimensions compared with the 'slow' subsystem. This technique was applied to analyse the explosion of a polydisperse spray of Diesel fuel. Clear advantages were demonstrated from the point of view of accuracy and CPU efficiency when compared with the conventional approach widely used in CFD codes. The difference between the solution of the full and decomposed systems of equations was shown to be negligibly small for practical applications.

CONCLUSIONS

Recent developments in the models of droplet heating and evaporation were reviewed. In agreement with the previous study, the gas phase model suggested by Abramzon and Sirignano [15] was shown to be the most accurate and was recommended for application. A comparison of the performance of two liquid phase models was undertaken. These are the infinite thermal conductivity (ITC) model and the effective thermal conductivity (ETC) model. Following our earlier studies [17-19], the application of the latter model was based on the analytical solution of the heat conduction equation inside droplets. Both the ITC and ETC liquid phase models and several gas phase models, including the one suggested in

[15], were implemented into a customised version of the KIVA II computational fluid dynamics (CFD) code. When modelling the radiative heating, the semi-transparency of the droplets was taken into account, but not the effects of spatial distribution of the radiation absorption. The model originally suggested in [21] was used to simulate this effect. Autoignition was modelled based on the Shell autoignition model and three spray break-up models were used: the conventional TAB and WAVE spray break-up models and the modified version of the WAVE model in which the effects of jet acceleration at the initial stage of spray development are taken into account. The results of investigation of the ignition delay in Diesel engines, using this code, were presented. The results of computations show a reasonably good agreement with in-house experimental data referring to autoignition delay. In-cylinder pressures from 5 to 9 MPa and injection pressure 160 MPa were used. In agreement with our previous results based on a zero-dimensional in-house CFD code, the effective thermal conductivity model predicts smaller ignition delay than the infinite thermal conductivity model. Both models predict decreasing ignition delay with increasing in-cylinder pressure, in agreement with experimental measurements. In agreement with the previously obtained results, the effect of the choice of gas model on ignition delay was shown to be small. Some recent non-traditional developments of the models referring to droplet heating and evaporation were briefly summarised. These are the model based on the coupled solution for the liquid and gas phase, the kinetic model of evaporation, and the dynamic decomposition technique for the solution of ordinary differential equations describing droplet heating and evaporation and the ignition of the fuel vapour/air mixture.

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