# Advanced models for droplet heating and evaporation: effect on the autoignition of diesel fuel sprays

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### **Abstract**

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, are reviewed. To describe properties of 'hot' diesel fuel sprays, new sub-models for spray breakup, droplet heating and evaporation and Shell autoignition were implemented into the KIVA II CFD code. To validate these models, the autoignition of diesel sprays was investigated experimentally at in-cylinder pressures from 5 to 9 MPa and injection pressures from 100 to 160 MPa. The sensitivity of predicted evaporation time and ignition delay to the choice of models is discussed.

## Introduction

Modelling of the autoignition of Diesel fuel sprays is expected to take into account a number of processes, including the dynamics and breakup of sprays, heating and evaporation of individual droplets and autoignition of the fuel vapour/air mixture in realistic three dimensional enclosures [1]. 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 [2]. 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 (see [2]). Droplet heating was typically modelled based on the assumption that the thermal conductivity of droplets is infinitely high [2]. 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. In this paper, the focus will be on the further development of droplet heating and evaporation models and their effect on the modelling of the autoignition of Diesel fuel

Bertoli and Migliaccio [3] 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. These include the parabolic temperature profile model [4-5] and those based on the analytical solution of the heat conduction equation inside droplets [6,7]. 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 [8-11]. 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. It took into account the coupling between the liquid and gas phases and described the autoignition process based on the eight step chain branching reaction scheme (Shell model) [12-14]. 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 zerodimensional 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 [7], and more accurate than the solution based on the parabolic temperature profile mode [7,8]. 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 of radiation absorption inside droplets (cf. [16,17]). It was pointed out that in the absence of breakup, the influence of the temperature gradient inside droplets on droplet evaporation under realistic diesel

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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 and evaporation processes, and the ignition of the evaporated fuel/air mixture.

In this paper the models of droplet heating and evaporation, developed at the University of Brighton, are reviewed and applied to modelling Diesel fuel spray autoignition, using the customised version of CFD code KIVA II. The results of modelling are validated against in-house experimental data where appropriate.

## **Specific Objectives**

- 1. Review of models of droplet heating and evaporation, relevant to Diesel engine applications.
- 2. Application of some of these models to simulation of the autoignition process in realistic Diesel engine conditions.
- 3. Validation of the results of modelling against in-house experimental data.

## **Models of Droplet Heating and Evaporation**

The liquid phase models actually used in CFD codes or 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 [11]:

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

where  $T_{s0}$  and  $T_g$  are the initial droplet temperature and ambient gas temperature respectively,  $c_l$  and  $\rho_l$  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 [11]:

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

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:

$$h(T_g - T_s) = -\rho_l L \frac{dR_d}{dt} + k_l \frac{\partial T}{\partial R} \Big|_{R=R_d},$$
 (3)

where L is the latent heat of evaporation, effects of swelling are ignored at this stage, 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).

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]:

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

The solution to Equation (2) for h=const can be presented as [7]:

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

$$-\frac{\sin \lambda_{n}}{\lambda_{n}^{2} \left\|V_{n}\right\|^{2}} \int_{0}^{1} \frac{d\mu_{0}(\tau)}{d\tau} \exp\left[-\kappa_{0} \lambda_{n}^{2} (t-\tau)\right] d\tau \right\} \sin\left(\frac{\lambda_{n} R}{R_{d}}\right)$$

$$+\frac{R_d}{R}\sum_{n=1}^{\infty} \frac{p_n}{\kappa_0 \lambda_n^2} \left[ 1 - \exp(-\kappa_0 \lambda_n^2 t) \right] \sin\left(\frac{\lambda_n R}{R_d}\right)$$
 (5)

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,  $\overline{T} = RT_{d0}(R)/R_d$ ,  $\kappa_0 = k_l/(c_l\rho_lR_d^2)$ ,  $\lambda_n$  are solutions to the equation:

$$\lambda_n \cos \lambda_n + h_0 \sin \lambda_n = 0,$$

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

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

$$p_{n} = \frac{1}{\|V_{n}\|^{2}} \int_{0}^{1} \left[ \frac{RP(t,R)}{R_{d}} \right] V_{n}(R) d(R/R_{d}).$$

Ignoring the dependence of the distribution of thermal radiation absorption on R and t, we can present the expression for P(R) as [16-18]:

$$P(R) = \frac{3\sigma}{\rho_{l}c_{l}} aR_{d}^{b-1}T_{ext}^{4},$$
 (6)

where we assumed that the radiation temperature  $\theta_R$  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  $5 \le R_d \le 50 \, \mu \text{m}$  and  $1000 \le T_{ext} \le 3000 \, \text{K}$  is provided by the functions [17]:

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

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

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  $k_{\text{eff}} = \chi k_l$ , where the coefficient  $\chi$  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 (5) was incorporated into a numerical code [9,10].

The values of h are controlled by the conditions in the gas phase. 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:

$$\frac{dR_d}{dt} = -\frac{k_g Sh}{2\rho_l c_{pg} R_d},\tag{7}$$

where  $k_g$  is the gas thermal conductivity,  $c_{pg}$  is the gas specific heat capacity at constant pressure, Sh is the Sherwood number. 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 [10].

Model 0:

$$Nu = 2\frac{\ln(1+B_M)}{B_M} \left(1 + 0.3 \operatorname{Re}_d^{1/2} \operatorname{Pr}_d^{1/3}\right)$$
  

$$Sh = 2\ln(1+B_M) \left(1 + 0.3 \operatorname{Re}_d^{1/2} \operatorname{Sc}_d^{1/3}\right)$$

where  $B_M$  is the Spalding mass number,  $\mathrm{Re}_d$ ,  $\mathrm{Pr}_d$ ,  $\mathrm{Sc}_d$  are Reynolds (based on droplet diameter), Prandtl and Schmidt numbers respectively.

Model 1

$$Nu = 2\frac{\ln(1+B_T)}{B_T} \left(1 + 0.3 \operatorname{Re}_d^{1/2} \operatorname{Pr}_d^{1/3}\right)$$
  

$$Sh = 2\ln(1+B_M) \left(1 + 0.3 \operatorname{Re}_d^{1/2} Sc_d^{1/3}\right)$$

where  $B_T$  is the Spalding heat transfer number.

Model 2:

$$Nu = 2 \frac{\ln(1 + B_T)}{B_T} \left( 1 + 0.3 \operatorname{Re}_d^{1/2} \operatorname{Pr}_d^{1/3} / F(B_T) \right)$$
  

$$Sh = 2 \ln(1 + B_M) \left( 1 + 0.3 \operatorname{Re}_d^{1/2} \operatorname{Sc}_d^{1/3} / F(B_M) \right),$$
  
where

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

Model 3:

$$Nu = 2 \frac{\ln(1 + B_T)}{B_T} (1 + \frac{1}{2} [(1 + \text{Re}_d \text{ Pr}_d)^{1/3}]$$

$$\max[1, \text{Re}_d^{0.077}] - 1])$$

$$Sh = 2 \frac{\ln(1 + B_M)}{B_M} (1 + \frac{1}{2} [(1 + \text{Re}_d Sc_d)^{1/3}]$$

$$\max[1, \text{Re}_d^{0.077}] - 1]).$$

Model 4:

$$Nu = 2 \frac{\ln(1 + B_T)}{B_T} (1 + [(1 + \text{Re}_d \text{ Pr}_d)^{1/3})$$

$$\max[1, \text{Re}_d^{0.077}] - 1] / [2F(B_T)]])$$

$$Sh = 2 \frac{\ln(1 + B_M)}{B_M} (1 + [(1 + \text{Re}_d Sc_d)^{1/3})$$

$$\max[1, \text{Re}_d^{0.077}] - 1] / [2F(B_B)]]).$$

Model 5:

$$Nu = 2 \frac{\ln(1 + B_T)}{B_T} \left( 1 + 0.276 \operatorname{Re}_d^{1/2} \operatorname{Pr}_d^{1/3} / F(B_T) \right)$$
  

$$Sh = 2 \ln(1 + B_M) \left( 1 + 0.276 \operatorname{Re}_d^{1/2} \operatorname{Sc}_d^{1/3} / F(B_M) \right)$$

Model 6:

$$Nu = \frac{2 + 0.57 \operatorname{Re}_{d}^{1/2} \operatorname{Pr}_{d}^{1/3}}{(1 + B_{F})^{0.7}}$$
$$Sh = 2 \frac{1 + 0.435 \operatorname{Re}_{d}^{1/2} \operatorname{Sc}_{d}^{1/3}}{(1 + B_{M})^{0.7}},$$

where

$$B_F = \frac{c_{pf}(T_g - T_s)}{L} \left( 1 - \frac{Q_L}{Q_c} \right),$$

 $Q_c$  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. As shown in [10], gas phase model 4 predicts the evaporation time closest to the one based on the approximation of experimental data. This gas phase model, originally suggested in [15], was recommended for practical application in CFD codes. In most cases, the droplet evaporation time depends strongly on the choice of gas phase model. The dependence of this time on the choice of liquid phase model, however, is weak if the droplet break-up processes are not taken into account. On the other hand, the dependence of the droplet surface temperature, at the initial stage of heating and evaporation, on the choice of gas phase model is weak, while its dependence on the choice of liquid phase model is strong [10].

In Diesel engines, the processes of droplet heating and evaporation are followed by the autoignition of the fuel vapour/air mixture. The latter process is described by the above mentioned Shell model [13]. The application of this model to Diesel engines has been reported in numerous papers including [2, 19-22]. This study analyses the sensitivity of autoignition computations to the choice of the liquid and gas phase models, using various models of spray break-up.

The models described above for droplet heating and evaporation were implemented into a customised version of the KIVA-II Computational Fluid Dynamics (CFD) code [23] alongside the Taylor-analogy break-up (TAB) model (the default model in KIVA-II), and the conventional and modified version of the WAVE break-up model [25]. 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:

$$B_1 = B_1^{eq} + 3.8 \cdot \left(a^+\right)^{0.2},\tag{8}$$

where  $B_1^{eq} = 10$  is the break-up time of the conventional WAVE model [26], and  $a^+$  is a dimensionless acceleration parameter. This empirical equation has been suggested to describe better the highly transient initial stage of spray penetration. In all cases, the blob injection method was used [26]. In the Shell model, the pre-exponential constant for the reaction rate for the production of the branching agent was set to value  $A_{f4} = 3 \cdot 10^6$  [2].

The results of calculations have been 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 in the next section.

# **Experimental Setup**

In order to record the autoignition process, two high-speed CCD video cameras recording 27000 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 3000 ISO. In order to further maximise the sensitivity of the recordings, the lens was set to its widest aperture (f/1.9). Recordings were performed at three injection pressures (100 MPa, 140 MPa and 160 MPa), and a range of incylinder pressures (from 5 to 9 MPa).

In order to assess the time delay between the actual start of the injection and the start of the video recording, a light-emitting diode (LED) was linked to the injector pulse signal and positioned within the field of view of one of the cameras. The start of the video recordings and the start of the injection pulse (as represented by the LED) matched. Hence, these two events were separated by less than 0.04 ms (exposure time for 1 frame), and can be assumed coincident. The times at which the first fuel droplets were seen leaving the nozzle were measured to be 0.45 ms, 0.39 ms and 0.37 ms after the start of the recording for injection pressures of 100 MPa, 140 MPa and 160 MPa, respectively. The data have been adjusted to compensate for this delay.

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 was injected under pressure 160 MPa into the compressed air at pressures of 5, 6, 7.2 and 8.5 MPa and temperature close to 800 K. The injection duration was about 0.2 ms. The rate of injection was measured as a function of time using the Bosch-type technique [27]. In experiments, the ignition delay time was defined as a time period from the start of injection to the moment of appearance of a visible flame on video-recordings of the spray.

## 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 and spray break-up models. Gas model 4 was used for the analysis, following [10].

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 axisymmetric 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 in the domain during the injection pulse was set to 1000.

The predicted and experimentally measured ignition delays of Diesel sprays are shown in Figures 1 and 2.

Figure 1 shows variation of the ignition delay time predicted using various spray break-up models, the ETC liquid heating model and gas-phase model 4. As follows from this figure, 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 [2]. Thus, the TAB model predicts faster spray atomisation and shorter ignition delays, in comparison with the conventional and modified WAVE models.

Figure 1 shows that the ignition delay curves for the modified and conventional WAVE models 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 (~2ms), 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  $A_{f4} = 3 \cdot 10^6$ .

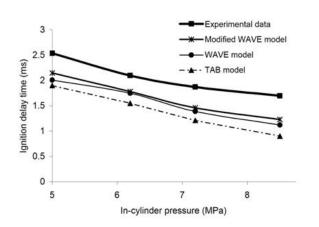


Figure 1. Predicted and experimentally measured ignition delay times versus in-cylinder pressure for various spray break-up models. 1000 droplet parcels with initial droplet temperature 400 K was injected into a cylinder with initial temperature 800 K. The ETC liquid phase model and gas model 4 were used.

Figure 2 shows the effect of the liquid-phase model (ETC and ITC) on the ignition delay time. As follows from this figure, the choice of liquid phase model can significantly affect the predictions of autoignition delay. 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 [10], the ignition delay predicted by the ETC model is always less than the one predicted by the ITM. As in the case of Figure 1, the model is not expected to predict exact coincidence between predicted and measured ignition

delays due to a rather arbitrary choice of the parameter  $A_{\it f4}$  .

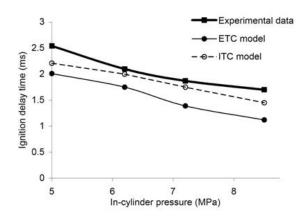


Figure 2. Predicted and experimentally measured ignition delay times versus in-cylinder pressure for ETC and ITC liquid-phase models. 1000 droplet parcels with initial droplet temperature 400 K was injected into a cylinder with initial temperature 800 K. The conventional WAVE spray break-up model and gas model 4 were used.

### **Conclusions**

Preliminary results are presented of an investigation into the effects of droplet heating and evaporation models on the predicted autoignition delay of Diesel sprays. Based on our previous study, the gas phase model suggested by Abramzon and Sirignano [15] was used. A comparison of the performance of two liquid phase models was undertaken. These are the infinite thermal conductivity model and the effective thermal conductivity model. Following our earlier studies [7,10], the application of this model was based on the analytical solution of the heat conduction equation inside droplets. The testing was performed for 3 spray break-up models: 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. All these models have been implemented into a customised version of the KIVA II CFD code. 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 zerodimensional in-house code, the effective thermal conductivity model predicts smaller ignition delay than the infinite thermal conductivity model. Both models predict decreasing ignition delay with increasing incylinder pressure, in agreement with experimental measurements.

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