

# Modelling of heating, evaporation and ignition of fuel droplets: combined analytical, asymptotic and numerical analysis

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## **Abstract.**

The paper discusses recent progress in the development of a combined analytical, asymptotic and numerical approach to modelling of heating and evaporation of fuel droplets and ignition of a fuel vapour/ air mixture. This includes a new approach to combined analytical and numerical modelling of droplet heating and evaporation by convection and radiation from the surrounding hot gas. The relatively small contribution of thermal radiation to droplet heating and evaporation allows us to take it into account using a simplified model, which does not consider the variation of radiation absorption inside droplets. The results of the analysis of the simplified problem of heating and evaporation of fuel droplets and ignition of fuel vapour/ air mixture based on the asymptotic method of integral manifolds are discussed. The semi-transparency of droplets was taken into account in this analysis, and a simplified model for droplet heat-up was used. The results of investigations of the effect of the temperature gradient inside fuel droplets on droplet evaporation, break-up and the ignition of fuel vapour/ air mixture based on a new zero-dimensional code are reviewed. The convection heating of droplets is described in this code based on a combined analytical and numerical approach. A new decomposition technique for a system of ordinary differential equations, based on the geometrical version of the integral manifold method is discussed. This is based on comparing the values of the right hand sides of these equations, leading to the separation of the equations into 'fast' and 'slow' variables. The hierarchy of the decomposition is allowed to vary with time. The application of this technique to analyse the explosion of a polydisperse spray of diesel fuel is presented. It is pointed out that this approach has clear advantages from the point of view of accuracy and CPU efficiency when compared with the conventional approach widely used in CFD codes.

## **1. Introduction**

The problems of droplet heating, evaporation and ignition of fuel vapour/ air mixture have been widely discussed in the literature [1] - [10]. However, the models used in most practical engineering applications tend to be rather simple. This is due to the fact that droplet heating and evaporation have to be modelled alongside the effects of turbulence, combustion, droplet break-up and related phenomena in realistic 3D enclosures. Hence, finding a compromise between the complexity of the models and their computational efficiency is the essential precondition for successful modelling. In a series of our recent papers [11] - [25] an attempt was made to develop simplified models for droplet heating, evaporation and ignition of fuel vapour/air mixture;

the sophisticated underlying physics was described using relatively simple mathematical tools (analytical solutions and asymptotic analysis). Some of these models, including those taking into account the effects of temperature gradient inside droplets, recirculation inside them and their radiative heating, were implemented into numerical codes focused on simulating droplet heating, evaporation and ignition of fuel vapour /air mixture [21, 23]. This work effectively focused on the development of a combined analytical, asymptotic and numerical approach to modelling of the whole process. Although the work in this direction is far from complete, some progress has been made. The main objective of this paper is to present a brief overview of the relevant results reported in [11] - [25].

The main equations and approximations used for the numerical analysis of the problem are summarised in Section 2. The new approach to combined analytical and numerical modelling of droplet heating and evaporation is discussed in Section 3. In Section 4 the results of asymptotic analysis of heating and evaporation of fuel droplets and the ignition of fuel vapour/ air mixture are discussed. The combined analytical and numerical analysis of these processes is discussed in Section 5. The analyses of the same processes based on combined asymptotic and numerical approaches are discussed in Section 6. The main results of the paper are summarised in Section 7.

## 2. Basic equations for spray modelling

Numerical spray modelling is traditionally based on the Lagrangian approach coupled with the Eulerian representation of the gas phase. This permits the decomposition of complicated and highly nonlinear systems of PDEs, describing interactions between computational cells, and the systems of ODEs that govern processes in individual computational cells, including liquid/gas phase exchange and chemical kinetics. The systems of ODEs are usually integrated using much shorter time steps  $\delta t$  than the global time steps used for calculating the gas phase  $\Delta t$ . In this section, basic ODEs used for modelling droplet heating, evaporation and combustion will be summarised [21]. These equations will be presented in their general form, following [4, 5, 9]. A number of processes, including droplet dynamics, break-up and coalescence, and the effects of temperature gradient inside droplets will be ignored at this stage. These will be discussed briefly later in Sections 3 and 5. Also, equations will be presented for stationary droplets. The generalization of these equations for moving droplets is discussed in a number of papers and books, including [5, 9].

### *Droplet mass*

As shown in [5], the equation for a stationary droplet mass  $m_d$  can be written as:

$$\frac{dm_d}{dt} = -4\pi \frac{\bar{k}_g R_d}{c_{pF}} \ln(1 + B_T), \quad (1)$$

where

$$B_T = \frac{c_{pF}(T_g - T_s)}{L_{\text{eff}}}$$

is the temperature Spalding number, and

$$L_{\text{eff}} = L(T_s) + Q_L / \left( \frac{dm_d}{dt} \right),$$

where  $L$  is the specific latent heat of vaporization,  $Q_L$  is the heat spent on droplet heating,  $\bar{k}_g$  is the average gas thermal conductivity,  $R_d$  is the droplet radius,  $c_{pF}$  is the specific heat capacity of fuel vapour, and  $t$  is time.

An alternative form of the equation for  $m_d$  can be written as [4, 9]:

$$\frac{dm_d}{dt} = -4\pi\rho_{\text{total}}D_gR_d \ln(1 + B_M), \quad (2)$$

where  $D_g$  is the binary diffusion coefficient for fuel vapour in the ambient gas,  $\rho_{\text{total}}$  is the total gas density,  $B_M = (Y_{fs} - Y_{f\infty})/(1 - Y_{fs})$  is the Spalding mass number,  $Y_{fs}$  and  $Y_{f\infty}$  are the mass fractions of fuel vapour near the droplet surface and in the ambient gas respectively. The expression for  $Y_{fs}$  can be written as:

$$Y_{fs} = \left[ 1 + \left( \frac{p}{p_{Fs}} - 1 \right) \frac{M_a}{M_f} \right]^{-1},$$

where  $p$  and  $p_{Fs}$  are the ambient pressure and the pressure of saturated fuel vapour near the surface of droplets respectively;  $M_a$  and  $M_f$  are molar masses of air and fuel;  $p_{Fs}$  can be calculated from the Clausius–Clapeyron equation, see [4]:

$$p_{Fs} = \exp \left[ a_f - \frac{b_f}{T_s - 43} \right], \quad (3)$$

where  $a_f$  and  $b_f$  are constants to be specified for specific fuels,  $T_s$  is the surface temperature of fuel droplets in K;  $p_{Fs}$  given by Equation (3) is in kPa. In many applications it is assumed that  $Le=1$ , and the temperature dependence of liquid density, gas thermal conductivity and viscosity is ignored. The values  $a_f = 15.5274$  and  $b_f = 5383.59$  are recommended for diesel fuel [4].

#### *Droplet temperature*

Following [5, 11, 15] we can write the equation for the stationary droplet temperature as:

$$m_d c_l \frac{dT_d}{dt} = 4\pi R_d^2 h (T_g - T_d) - \dot{m}_d L + 4\pi R_d^2 \sigma \bar{Q}_a \theta_R^4, \quad (4)$$

where

$$\text{Nu} = \frac{2hR_d}{k_g} = 2 \frac{\ln(1 + B_T)}{B_T}.$$

Here  $\theta_R$  is the radiative temperature, as calculated from the P-1 model ( $\theta_R = T_{\text{ext}}$  (external temperature) for optically thick gases and  $\theta_R = T_g$  for optically thin gases),  $\bar{Q}_a$  is the average absorption efficiency factor, which can be calculated from the equation [11, 15]:

$$\bar{Q}_a = a_r R_d^{b_r}, \quad (5)$$

where  $a_r$  and  $b_r$  are polynomials in  $\theta_R$  (explicit expressions for several types of diesel fuel are given in [15]),  $c_l$  is the liquid specific heat capacity.  $L$  depends on temperature in the general case.

In Equations (4) and (5) the effects of temperature gradient and the distribution of thermal radiation inside droplets are ignored. These will be discussed later in Section 3. Equations (1) (or (2)) and (4), written for individual droplets, are applied to describe droplet parcels, following the conventional approach widely used in computational fluid dynamics codes.

### Fuel vapour density

The equation for fuel vapour density ( $\rho_{fv}$ ) follows directly from the conservation of fuel vapour:

$$\alpha_g \frac{d\rho_{fv}}{dt} = -\alpha_g CT + \left[ \sum_i \dot{m}_{di} / V \right], \quad (6)$$

where  $\alpha_g$  is the volume fraction of gas assumed equal to 1 in most cases, the summation is assumed over all droplets in volume  $V$ ,  $Q_f$  is the heat released per unit mass of burnt fuel vapour (in J/kg), and  $CT$  is the chemical term describing fuel depletion (in kg/(m<sup>3</sup>s)).

Following [26] the expression for the rate of reaction is

$$k_{cr} = A[\text{fuel}]^a [O_2]^b \exp[-E/(BT)],$$

where  $k_{cr}$  has units of mole/(cm<sup>3</sup>·s), while the concentrations of fuel [fuel] and oxygen [ $O_2$ ] has units of mole/cm<sup>3</sup>. The values of these coefficients given for C<sub>10</sub>H<sub>22</sub> are the closest to those of n-dodecane (C<sub>12</sub>H<sub>26</sub>) (the closest approximation for diesel fuel) [26]:

$$A = 3.8 \times 10^{11} \frac{1}{s} \left( \frac{\text{mole}}{\text{cm}^3} \right)^{1-a-b} = 2.137 \times 10^9 \frac{1}{s} \left( \frac{\text{kmole}}{\text{m}^3} \right)^{1-a-b};$$

$$E = 30 \frac{\text{kcal}}{\text{mole}} = 1.255 \times 10^8 \frac{\text{J}}{\text{kmole}}; \quad a = 0.25; \quad b = 1.5.$$

Using  $A$  in units of  $\frac{1}{s} \left( \frac{\text{mole}}{\text{cm}^3} \right)^{1-a-b}$  and  $E$  in units of  $\frac{\text{J}}{\text{kmole}}$ , we can write:

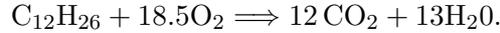
$$CT = A M_{O_2}^{-1.5} M_f^{0.75} \rho_{fv}^{0.25} \rho_{O_2}^{1.5} \exp[-E/(BT)],$$

where  $M_{O_2} = 32$  kg/kmol, and  $M_f = 170$  kg/kmol are molar masses of oxygen and fuel respectively in kg/kmole,  $\rho_{O_2}$  is the density of oxygen.

In the case of diesel engines,  $CT$  is usually calculated based on the so called Shell model [27, 28, 29].

### Density of oxygen

We assume that the fuel is n-dodecane. A single step global reaction for n-dodecane combustion can be written as:



Hence the equation for the density of oxygen is

$$\frac{d\rho_{O_2}}{dt} = -18.5 \frac{M_{O_2}}{M_f} CT = -3.48235 CT. \quad (7)$$

A useful characteristic, widely used as a measure of reactivity of the fuel vapour /air mixture, is the equivalence ratio:

$$\varphi = \frac{\text{Fuel}/\text{Air}}{(\text{Fuel}/\text{Air})_{\text{stoich}}} = \frac{\text{Fuel}/\text{Oxygen}}{(\text{Fuel}/\text{Oxygen})_{\text{stoich}}} = \frac{18.5 \times 32}{170} \frac{\rho_{fv}}{\rho_{O_2}} = \frac{3.48 \rho_{fv}}{\rho_{O_2}},$$

where  $(\text{Fuel}/\text{Air})_{\text{stoich}}$  is the stoichiometric ratio of the densities of fuel and air.

### Gas temperature

The condition of energy balance leads us to the following equation for the gas temperature:

$$c_{\text{mix}}\rho_{\text{mix}}\frac{dT_g}{dt} = \alpha_g Q_f \text{CT} - \left[ \sum_i m_{di} c_l \frac{dT_{di}}{dt} + \sum_i \dot{m}_{di} L + \sum_i \dot{m}_{di} c_{pF} (T_g - T_{di}) \right] / V, \quad (8)$$

where the summation is performed over all droplets in the volume  $V$  [21].

### 3. Heating of droplets

As already mentioned, in most practical engineering applications in CFD (Computational Fluid Dynamics) codes only rather simple models for droplet heating have been used. These models have been based on the assumption that the thermal conductivity of liquid is infinitely high and the temperature gradients inside droplets can be ignored (see e.g. [30, 29, 31]). These assumptions were used for deriving Equation (4). This simplification of the model was required due to the reasons discussed in the Introduction. Bertoli and Migliaccio [32] were perhaps the first who drew attention to the fact that the accuracy of CFD computations of heating, evaporation and combustion of diesel fuel sprays could be substantially 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 is added to the solution of other equations in a CFD code. Although this approach is expected to increase the accuracy of CFD predictions, the additional computational cost might be too high for practical applications.

An alternative approach to taking into account the effects of finite thermal conductivity and recirculation inside droplets has been suggested in [12]. This model is based on the parabolic approximation of the temperature profiles inside the droplets. This approximation does not satisfy the heat conduction equation with appropriate boundary conditions, but satisfies the equation of thermal balance at the droplet surfaces. Comparison with numerical solutions of the transient problem for moving droplets shows the applicability of this approximation to modelling the heating and evaporation processes of fuel droplets in diesel engines. The simplicity of the model makes it particularly convenient for implementation into multidimensional CFD codes to replace the abovementioned model of isothermal droplets. Preliminary results of the implementation of the simplified version of this model into a research version of the CFD code VECTIS of Ricardo Consulting Engineers was demonstrated in [33].

Instead of solving the heat conduction equation numerically inside a droplet, or using a simplified model based on the parabolic approximation, one could think about the development of a numerical code based on the analytical solutions of this equation. A number of analytical solutions have been obtained and discussed in [34]–[37] and [18]. In most cases these analytical solutions have been presented in the form of convergent series.

The finite liquid thermal conductivity models were generalised to take into account the internal recirculation inside droplets. This was achieved by replacing the thermal conductivity of the liquid  $k_l$  by the so called effective thermal conductivity  $k_{\text{eff}} = \chi k_l$ , where the coefficient  $\chi$  varies from about 1 (at droplet Peclet number  $\text{Pe}_d = \text{Re}_d \text{Pr}_d < 10$ ) to 2.72 (at  $\text{Pe}_d > 500$ ). It can be approximated as [5]  $\chi = 1.86 + 0.86 \tanh [2.225 \log_{10} (\text{Pe}_d/30)]$ . The values of transport coefficients in  $\text{Pe}_d$  are taken for the liquid fuel, the relative velocity of droplets is taken for the calculation of  $\text{Re}_d$ . This model can predict the droplet average surface temperature, but not the distribution of temperature inside droplets. In our case, however, we are primarily interested in the accurate prediction of the former temperature, which controls droplet evaporation. Hence, the applicability of this model can be justified.

In the rest of this section the analytical solution of the heat transfer problem inside a droplet and its implementation into a numerical code will be discussed based on the results reported in [18, 19].

Assuming that droplet heating is spherically symmetric, the transient heat conduction equation inside this droplet can be written as [34]:

$$c_l \rho_l \frac{\partial T}{\partial t} = k_l \left( \frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right) + P_1(R), \quad (9)$$

where  $\rho_l$  is the liquid density,  $T = T(R, t)$  is the droplet temperature,  $R$  is the distance from the centre of the droplet and  $P_1(R)$  is the power generated in unit volume inside the droplet due to external radiation. While  $c_l$ ,  $\rho_l$  and  $k_l$  are assumed to be constant for the analytical solution of Equation (9), their variations with temperature and time were accounted for when the analytical solutions were incorporated into the numerical code.

Assuming that the droplet is heated by convection from the surrounding gas, and cooled due to evaporation, the energy balance equation at the droplet surface can be written as:

$$h(T_g - T_s) = -\rho_l L \dot{R}_d + k_l \left. \frac{\partial T}{\partial R} \right|_{R=R_d}, \quad (10)$$

where  $h = h(t)$  is the convection heat transfer coefficient (time dependent in the general case),  $R_d$  is the droplet's radius,  $T_g$  is the gas ambient temperature,  $T_s$  is the droplet's surface temperature,  $L$  is the specific heat of evaporation. We took into account that  $\dot{R}_d < 0$ . Equation (10) can be considered as the boundary condition for Equation (9) at  $R = R_d$ . This needs to be complemented by the boundary condition at  $R = 0$ :

$$\left. \frac{\partial T}{\partial R} \right|_{R=0} = 0.$$

The initial condition is taken in the form:  $T(t = 0) = T_0(R)$ .

The radiation term was given in two forms. Firstly, following [14] we can write:

$$P_1(R) = \frac{3\pi}{R_d} \int_{\lambda_1}^{\lambda_2} w(r, \lambda) Q_a B_\lambda(T_{\text{ext}}) d\lambda, \quad (11)$$

where  $r = R/R_d$ ,  $B_\lambda(T_{\text{ext}}) = C_1 / [\pi \lambda^5 [\exp(C_2/(\lambda T_{\text{ext}})) - 1]]$ ,  $C_1 = 3.742 \times 10^8 \frac{\text{W}\mu\text{m}^4}{\text{m}^2}$ ,  $C_2 = 1.439 \times 10^4 \mu\text{m} \cdot \text{K}$ ,  $\lambda$  is the wavelength in  $\mu\text{m}$ ,  $T_{\text{ext}}$  is the external temperature responsible for radiative heating which is assumed to be constant, and  $Q_a$  is the efficiency factor of absorption. The required approximation for  $Q_a$  depends on the specific application of the model. If this application is focused on the problem of heating and evaporation of diesel fuel droplets it can be approximated by [14, 38]:

$$Q_a = \frac{4n}{(n+1)^2} [1 - \exp(-2a_\lambda R_d)],$$

where  $a_\lambda$  is the liquid fuel absorption coefficient,  $n$  is the refractive index of liquid diesel fuel. We note that  $a_\lambda$  is related to the index of absorption  $\kappa_\lambda$  by  $\kappa_\lambda = a_\lambda \lambda / (4\pi)$ , and  $w(r, \lambda)$  is the normalised spectral power of radiation per unit volume absorbed inside the droplet. The following equations were used for  $w$  [14]:

$$w(r, \lambda) = \frac{[1 - \mu_* \Theta(r - 1/n)] (r^2 + \bar{\gamma})}{[0.6(1 - \mu_c^5) - \mu_c^3/n^2] + \bar{\gamma}(1 - \mu_c^3)}, \quad (12)$$

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

$$\Theta(x) = \begin{cases} 0 & \text{when } x < 0 \\ 1 & \text{when } x \geq 0 \end{cases},$$

or

$$w(\tau) = \frac{\xi^2 \tau_0^3}{3} \frac{\exp[-\xi(\tau_0 - \tau)]}{\tau_0(\xi\tau_0 - 2) + (2/\xi)[1 - \exp(-\xi\tau_0)]}, \quad (13)$$

where  $\tau = a_\lambda R$ ,  $\xi = 2/(1 + \mu_c)$ . Equation (12) was used when  $\tau_0 < n\sqrt{2.5}$ , otherwise Equation (13) was used.  $\lambda_1$  and  $\lambda_2$  describe the spectral range of thermal radiation which contributes to droplet heating.

If we ignore the distribution of thermal radiation absorption inside droplets then a much simpler approach can be used, as suggested in [11, 15]. This is based on Equation (5) and can be written in the form:

$$P_1(R) = 3 \times 10^6 a_r \sigma R_{d(\mu\text{m})}^{b_r-1} \theta_R^4, \quad (14)$$

where the radiation losses from the droplets were ignored. The expressions for the coefficients  $a_r$  and  $b_r$  in this formula for a typical automotive diesel fuel (low sulphur ESSO AF1313 diesel fuel) in the range of external temperatures 1000 – 3000 K were obtained from [15].

Equation (11) is certainly more accurate than (14), but its application requires much more CPU time than application of (14). Most of the CPU time is actually spent on calculating the integral over  $\lambda$  in (11). The most accurate calculation of this integral is based on all experimentally measured values of the absorption coefficient  $a_\lambda$  (4111 points) [19]. As follows from the analysis of [19], the reduction of the number of these points to just 58, allows us to reduce CPU time by almost two orders of magnitude with the introduction of an error of less than 10%. This error can be tolerated in most cases. The analysis of [14] was based on the results of measurements of  $\lambda$  in the ranges 0.5 – 1.1  $\mu\text{m}$  and 2.0 – 6.0  $\mu\text{m}$ , while the results reported in [18, 19] were based on the measurements in the range 0.2 – 6.0  $\mu\text{m}$ .

Equation (10) can be rearranged to:

$$T_{\text{eff}} - T_s = \frac{k_l}{hR_d} \left. \frac{\partial T}{\partial r} \right|_{r=1}, \quad (15)$$

where:

$$T_{\text{eff}} = T_g + \frac{\rho_l L \dot{R}_d}{h}.$$

Equation (15) is complemented by the boundary condition at  $R = 0$  and the initial condition mentioned above. The value of  $\dot{R}_d$  is controlled by fuel vapour diffusion from the droplet surface. For stationary droplets it can be found from Equation (1) or (2).

Equations (9) and (1) (or (2)) for droplets were complemented by the equations for a droplet trajectory, the temperature of the gas phase ( $T_g$ ) (Equation (8)), fuel vapour density ( $\rho_{fv}$ ) (Equation (6)) and oxygen density (Equation (7)) within the Lagrangian spray model [23]. This system of ODEs of the Lagrangian model equations can be coupled with the solution of PDE of the Eulerian gas model. This is the conventional way of modelling spray/gas interaction in a CFD framework. The focus of this section, however, will be on Equations (9) and (2) only. The evaporation model used in our analysis is similar to the one used in most CFD codes. It is based on the assumption that fuel vapour in the vicinity of fuel droplet surface is always saturated. More rigorous analysis of droplet evaporation would require a kinetic approach which is beyond the scope of this paper (see [16, 39]).

In the case when the convection heat transfer coefficient  $h(t) = \text{const}$ , the solution of Equation (9) with  $R_d = \text{const}$  and the corresponding boundary and initial conditions, as discussed above, is [18]:

$$T(r, t) = \frac{1}{r} \sum_{n=1}^{\infty} \left\{ \frac{p_n}{\kappa \lambda_n^2} + \exp[-\kappa \lambda_n^2 t] \left( q_n - \frac{p_n}{\kappa \lambda_n^2} \right) - \frac{\sin \lambda_n}{\|v_n\|^2 \lambda_n^2} \mu_0(0) \exp[-\kappa \lambda_n^2 t] - \right.$$

$$- \frac{\sin \lambda_n}{\|v_n\|^2 \lambda_n^2} \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp[-\kappa \lambda_n^2 (t - \tau)] d\tau \} \sin \lambda_n r + T_{\text{eff}}(t), \quad (16)$$

where:

$$\mu_0(t) = \frac{hT_{\text{eff}}(t)R_d}{k_l}, \quad h_0 = (hR_d/k_l) - 1, \quad \|v_n\|^2 = \frac{1}{2} \left( 1 + \frac{h_0}{h_0^2 + \lambda_n^2} \right) \quad \kappa = \frac{k_l}{c_l \rho_l R_d^2},$$

$$p_n = \frac{1}{\|v_n\|^2} \int_0^1 \tilde{P}(r)v_n(r)dr, \quad q_n = \frac{1}{\|v_n\|^2} \int_0^1 \tilde{T}_0(r)v_n(r)dr,$$

$$\tilde{P}(r) = rP(r), \quad \tilde{T}_0(r) = rT_0(R), \quad v_n(r) = \sin \lambda_n r \quad (n = 1, 2, \dots),$$

where the positive eigenvalues  $\lambda_n$ , numbered in ascending order ( $n = 1, 2, \dots$ ), are found from the eigenvalue equation:

$$\lambda \cos \lambda + h_0 \sin \lambda = 0.$$

If  $T_0(r)$  is twice differentiable, then the series in (16) converges absolutely and uniformly for all  $t \geq 0$  and  $r \equiv R/R_d \in [0, 1]$ .

Equation (9) was also analysed in the case of almost constant  $h$  and arbitrary  $h$  [18], but the results turned out to be of limited practical importance for implementation into CFD codes [19].

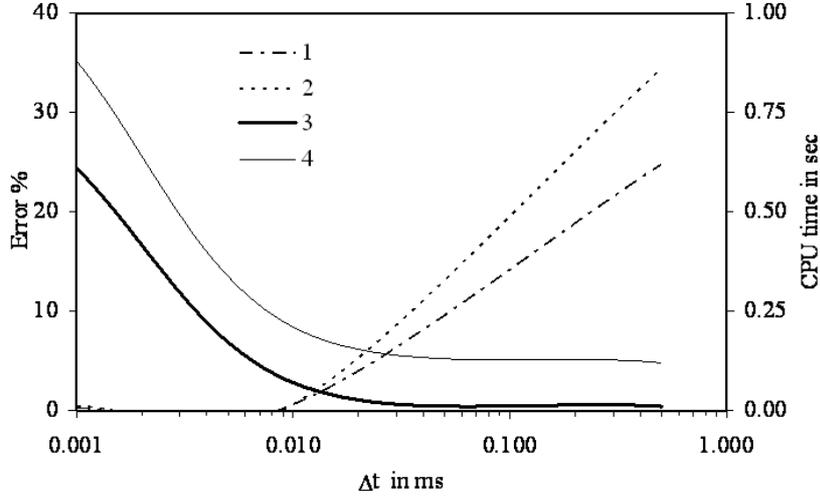
In the limiting case when  $\mu_0 = \text{const}$ ,  $P(r) = 0$ ,  $\dot{R}_d = 0$ ,  $T_{\text{eff}} = T_g = \text{const}$  and  $k_l \rightarrow \infty$  Equation (16) reduces to [37]:

$$T(t) \equiv T_d(t) = T_s(t) = T_g + (T_{s0} - T_g) \exp\left(-\frac{3ht}{c_l \rho_l R_d}\right). \quad (17)$$

Note that the value of  $T(t) \equiv T_d(t)$  does not depend on  $r$ . The same equation could be obtained directly from the energy balance equation at the surface of the droplet, assuming that there is no temperature gradient inside.

A comparison of the performance of the above schemes in numerical codes for parameters relevant to diesel engines will be briefly summarised. Full details can be found in [19]. The initial droplet radius was taken equal to 10  $\mu\text{m}$ , and its initial temperature equal to 300 K. The droplet swelling and the temperature dependence of  $k_l$  are taken into account. The effect of droplet break-up was not taken into account. It was assumed that the droplet relative velocity reduces from 0.45 m/s to zero over 1 ms – the situation relevant to diesel engines when air entrainment by a fuel spray is taken into account. Several algorithms describing the heating and evaporation of these droplets were studied. These included: the algorithm based on the analytical solution (16); the numerical solution of the discretised Equation (9); the performance of the numerical algorithm based on the parabolic temperature profile model; and the numerical algorithm based on the assumption that there is no temperature gradient inside the droplet (Equation (17)). It was assumed that  $T_g = 1000$  K; droplets were allowed to evaporate and swell.

It follows from the analysis in [19] that the predictions of the numerical solution of the discretised Equation (9) and the numerical calculations using the analytical solution for  $h = \text{const}$  almost coincide for both the surface temperature and droplet radius when the time step was taken small enough ( $10^{-6}$  s). For the numerical solution of Equation (9), 1000 nodes along the droplet radius were used. Both these solutions differed noticeably from the predictions of the model based on the assumption of no temperature gradient inside the droplet. The predictions of the parabolic model were between these solutions. This means that from the point of view of accuracy the numerical solution of the discretised Equation (9) and the solution based on the algorithms using the solution for  $h = \text{const}$  were practically identical and superior to the



**Figure 1.** Plots of errors and CPU times from calculation of evaporation time versus time. The errors were calculated relative to the prediction of the numerical solution of the discretised heat conduction equation with  $\Delta t = 10^{-6}$  s and using 1000 nodes along the droplet radius (for the numerical solution of Equation (9)). The plots of errors are presented for the numerical algorithm based on the analytical solution for  $h = \text{const}$  (curves 1) and numerical solution of the discretised heat conduction equation (curves 2). Plots of CPU times are presented for the algorithm based on the analytical solution for  $h = \text{const}$  (curves 3) and numerical solution of the discretised heat conduction equation (curves 4). The effects of radiation are not taken into account [19].

numerical solutions based on the parabolic temperature profile model and the model with no temperature gradient inside the droplet.

The plots of errors and CPU times versus time step  $\Delta t$  for the numerical algorithm based on the analytical solution for  $h = \text{const}$  and numerical solution of the discretised heat conduction equation are shown in Fig. 1 [19]. 100 nodes along the radius were considered for the latter solution to provide calculations with relative errors of less than about 0.5%. The calculations for the parabolic temperature profile model and the numerical solution based on the assumption that there is no temperature gradient inside the droplet were performed using the adaptive time step. The errors from these calculations relative to the prediction of the numerical solution of the discretised heat conduction equation were 1.2% and 3.6% respectively [19]. All errors were calculated relative to the prediction of the numerical solution of the discretized heat conduction equation with 1000 nodes along the droplet radius and time step  $\Delta t = 0.001$  ms. As follows from Fig. 1, the errors from calculations based on the algorithm using the analytical solution for  $h = \text{const}$  were consistently lower when compared with the errors from calculations based on the numerical solution of the discretised heat transfer equation for  $\Delta t > 0.01$  ms. At smaller  $\Delta t$  these errors were close to zero for both solutions. This can be related to the fact that the numerical solution of the discretised heat conduction equation is based on the assumption that non-linear terms can, with respect to the time step, be ignored, while the algorithms using the analytical solution for  $h = \text{const}$  implicitly retain these terms.

Thus it can be concluded that Solution (16) is the most efficient for implementation into numerical codes [19]. Initially, this solution was applied at the first time step, using the initial distribution of temperature inside the droplet. The results of the analytical solution over this time step were used as the initial condition for the second time step etc. This approach was

compared with approaches based on the numerical solution of the discretised heat conduction equation (Equation (9)), those based on the assumption that there is no temperature gradient inside the droplet, and those based on the assumption that the temperature distribution inside the droplet has a parabolic profile. All these approaches were applied to the numerical modelling of fuel droplet heating and evaporation in conditions relevant to diesel engines, but without taking into account the effects of droplet break-up. The algorithm based on the analytical solution for constant  $h$  was shown to be more effective (from the point of view of the balance of accuracy and CPU time requirement) than the approach based on the numerical solution of the discretised heat conduction equation inside the droplet, and more accurate than the solution based on the parabolic temperature profile model. The relatively small contribution of thermal radiation to droplet heating and evaporation allowed the authors of [19] to describe it using a simplified model, which takes into account their semi-transparency, but does not consider the spatial variations of radiation absorption inside droplets (Equation (14)).

#### 4. Heating, evaporation and ignition of fuel droplets: asymptotic analysis

The previous section was primarily focused on the analysis of enhanced models for droplet heating. The general problem of heating and evaporation of droplets and ignition of fuel vapour/air mixture is based on the analysis of Equations (1) (or (2)), (4), (6), (7) and (8). Semenov [40] was perhaps the first to develop the basic theory of the phenomenon of thermal explosion, based on the solution of the simplified version of these equations. Since that time more and more complicated models have been suggested (see e.g. [7, 8]). They have been incorporated into various CFD packages and allowed to take into account heat and mass transfer and combustion processes in the mixture of gas and fuel droplets in a self-consistent way [30] – [31]. This approach, however, is not particularly helpful in aiding understanding of the relative contribution of various processes. An alternative approach to the problem is to analyze the equations in some limiting cases. This cannot replace CFD methods but can complement them. For example, the geometrical asymptotic method of integral manifolds can be used [41]. This method was successfully applied to modeling self-ignition problems [42] – [45]. In [30] it was applied to the specific problem of modeling the ignition process in diesel engines. These authors attempted to combine the asymptotic approach, based on the integral manifold method, and CFD simulations of the process, based on the CFD package VECTIS. The asymptotic analysis in this paper [30] took into account both convective and radiative heating of droplets, but it was assumed that the droplet temperature was constant (heat-up period was completed). The radiative heating model used was based on the assumption that fuel droplets are grey opaque spheres. Also, the chemical reaction term, used in the asymptotic model, was assumed in the one-step Arrhenius form. The latter might be a serious oversimplification as the combustion process in diesel engines involves hundreds of species and chemical reactions (see discussion in [29]). The analysis of these is beyond the capacity of most CFD codes and a number of reduced mechanisms were suggested [46] – [48]. One mechanism widely used in CFD codes is the so-called Shell model [27]. In [30] an attempt was made to approximate the contribution of the reduced chemistry, described by the Shell model, in the enthalpy equation in the Arrhenius form with the time-dependent pre-exponential factor  $A(t)$ . However, this had limited success as the function  $A(t)$  implicitly depended on fuel vapour and oxygen concentrations. The main argument supporting the application of the Arrhenius form of the chemical term was that the physical ignition delay for average sized droplets in diesel engines (due to heating and evaporation of droplets) is generally longer than the chemical ignition delay (due to chemical reactions [29]). The analysis of [24] was focused on further development of the model used in [30]. Firstly, the assumption that droplets are opaque gray spheres was replaced by a more realistic assumption that droplets are semi-transparent spheres with the average absorption efficiency factor approximated by a simplified version of Equation (5), assuming that the gas is optically thick (radiation temperature is equal

to gas temperature). Secondly, the process of droplet heat-up was taken into account using a simplified model. Thirdly, the equations were investigated for a wide range of parameters typical of diesel engines (not just average values as done in [30]). As in [30] the analysis was restricted to the case when the Spalding numbers  $B_M$  and  $B_T$  are well below 1. No deficiency of oxygen was not taken into account (Equation (7) was not considered). The remaining Equations (1) (or (2)), (4), (6) and (8) were written in the following simplified forms [24]:

$$\frac{dm_d}{dt} = -\frac{4\pi R_d^2}{L} (q_c + q_r) (1 - \zeta(T_d)), \quad (18)$$

$$m_d c_l \frac{dT_d}{dt} = 4\pi R_d^2 (q_c + q_r) \zeta(T_d), \quad (19)$$

$$\alpha_g \frac{dc_f}{dt} = -c_f \alpha_g A \exp\left(-\frac{E}{R_u T_g}\right) + \frac{4\pi R_d^2 n_d}{M_f L} (q_c + q_r) (1 - \zeta(T_d)), \quad (20)$$

$$c_{pg} \rho_g \alpha_g \frac{dT_g}{dt} = c_f \alpha_g Q_f M_f A \exp\left(-\frac{E}{R_u T_g}\right) - 4\pi R_d^2 n_d (q_c + q_r), \quad (21)$$

where  $c_f$  is the molar concentration of fuel vapour,  $M_f$  is the molar mass of fuel vapour (note that  $\rho_{fv} = c_f M_f$ ),  $q_c$  and  $q_r$  are convective and radiative heat fluxes,  $n_d$  is the number of droplets per unit volume (a monodisperse spray was considered),  $R_u$  is the universal gas constant,  $E$  is the activation energy in J/kmol. The parameter  $\zeta(T_d)$  takes into account the fraction of heat supplied from the gas which is spent on droplet heating. Following [49] it was taken in the form [24]:

$$\zeta(T_d) = \frac{T_b - T_d}{T_b - T_{d0}}, \quad (22)$$

where  $T_{d0}$  is the initial droplet temperature,  $T_b$  is the boiling temperature ( $\zeta(T_{d0}) = 1$ ;  $\zeta(T_b) = 0$ ).

As in [30], the asymptotic analysis of Equations (18) – (22) reported in [24] was based on method of integral manifolds. The focus of [24] was on the initial stage of the thermal explosion. Two main dynamical scenarios, depending on the initial concentration of the fuel droplets, were identified. These corresponded to two zones in the combustion chamber: the far zone (far from the droplet injector), where the initial droplet concentration is low, and the near zone (close to the droplet injector), where the initial droplet concentration is high. Note that the immediate vicinity of the nozzle, where liquid jet has not yet disintegrated into droplets, was beyond the scope of the analysis of [24].

In agreement with predictions of CFD calculations it was pointed out that the time of small (radii less or equal to 5  $\mu\text{m}$ ) droplet heating and evaporation in the far zone is smaller than the chemical ignition delay of the fuel vapor/air mixture [24]. Also, in agreement with CFD predictions, the total ignition delay was shown to decrease with increase of the initial gas temperature. In the near zone for large (radii greater or equal to 50  $\mu\text{m}$ ) droplets the process was shown to start with the fast initial gas cooling and slight heating of droplets. This was followed by a relatively slow heating of gas due to the chemical reaction and further droplet heating. The total ignition delay in the near zone was shown to be larger than in the far zone. It was expected that before a thermal explosion in the near zone takes place, the droplets breakup and are removed from this zone. Also, the whole process was shown to be likely affected by the explosion in the far zone [24]. In an optically thick gas the effects of thermal radiation were shown to be negligible for small droplets but were shown to be noticeable for large droplets. Some generalizations of the analysis of [24] were reported in [22]. These include the investigation of the effects of thermal radiation in optically thin gas, and the analysis was performed over a wide range of parameters.

## 5. Heating, evaporation and ignition of fuel droplets: combined analytical and numerical analysis

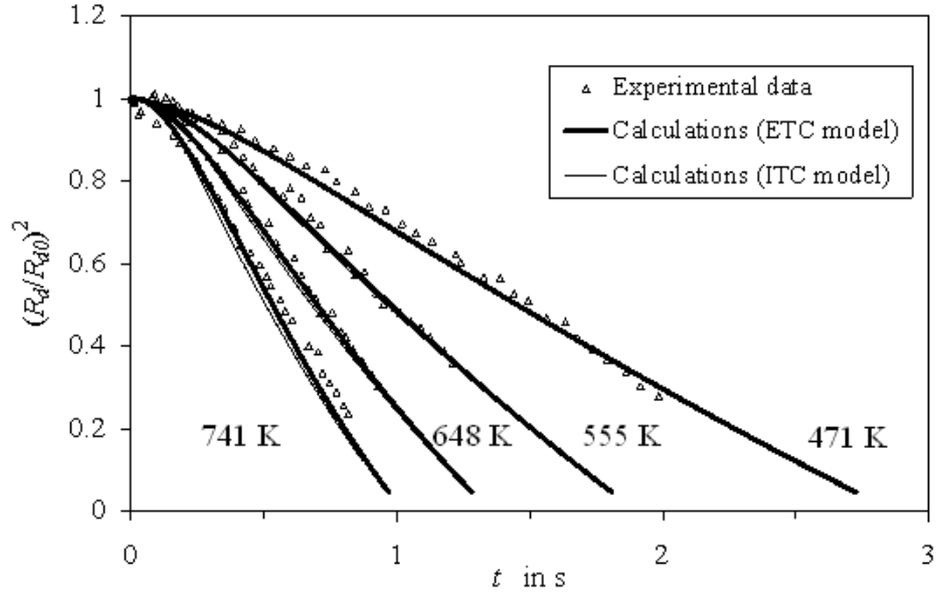
The results discussed in Section 3 refer to ‘one way’ heating of droplets by the surrounding gas. They cannot be used directly as predictive tools for studies of heating, evaporation and ignition of realistic fuel droplets. The analysis reported in [23] is focused on further development of the model described in Section 3, its testing and application to modelling the processes of heating, evaporation, ignition and break-up of diesel fuel droplets. In contrast to [19], the effect of droplet velocities, and the heating and evaporation on the surrounding gas were taken into account (coupled solutions). The surrounding gas was accelerated by the movement of the droplets. Then the gas was cooled with accompanying heating and evaporation of droplets. The fuel vapour was allowed to diffuse through the gas culminating in ignition of the fuel vapour/air mixture. These effects were expected to be accelerated significantly via droplet break-up [50] – [52]. The ignition process was modelled based on the Shell model mentioned above. The new model for droplet heating, described in Section 3, was implemented into a zero dimensional code in which all values of the gas parameters (velocity, temperature, fuel vapour concentration etc) are assumed to be homogeneous [23]. This conforms with the usual assumptions made in CFD codes regarding the individual cells.

Naturally, while the main focus of [23] was on the effects produced by the temperature gradients in droplets, a number of important processes were beyond its scope. These included the effects of real gases [53], near critical and supercritical droplet heating [54, 55], and analysis of droplet collision and coalescence [56, 57].

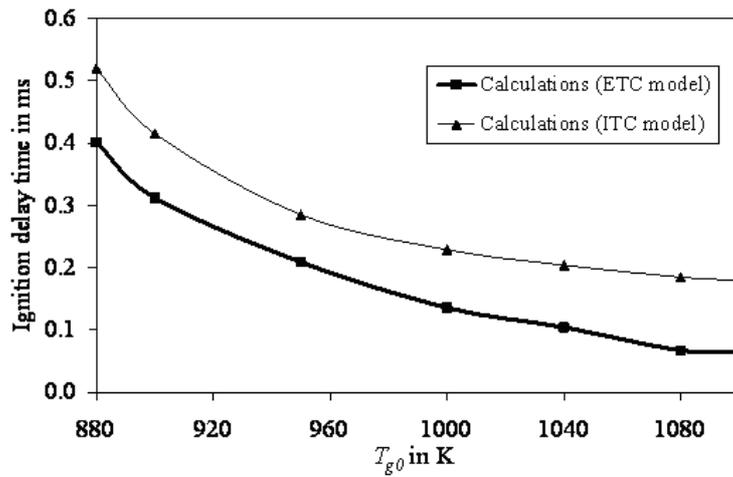
The predictions of the code developed in [23] were validated against experimental data published by Belardini et al [58], Nomura et al [59], and Tanabe et al [60]. In what follows a comparison between the experimental data reported in [59] and the predictions of the model will be discussed based on [23]. These data were obtained for suspended *n*-heptane droplets in a nitrogen atmosphere at pressures in the range between 0.1 and 1 MPa and temperatures in the range 400 K and 800 K. Initial droplet radii varied from 0.3 mm to 0.35 mm. The experiments were performed under microgravity conditions. The experimentally observed values of  $(R_d/R_{d0})^2$  versus  $t$  for pressure 0.1 MPa, initial gas temperatures 471 K, 555 K, 648 K, 741 K, and the initial droplet radii equal to 0.3 mm, are shown in Fig. 2. Also, the results of calculations based on the effective thermal conductivity (ETC) model, discussed earlier, and the infinite thermal conductivity (ITC) model (based on Equations (4) and (17)) for the same values of parameters are shown [23]. The physical properties of *n*-heptane used in the calculations are given in [23].

As follows from Fig. 2, both ITC and ETC models show good agreement with experimental data. For  $T_{g0} = 471$  K and  $T_{g0} = 555$  K the predictions of the models practically coincide. At higher temperatures, however, the predictions of the ETC model are in marginally better agreement with experimental data, compared with the ITC model, as expected. At lower initial gas temperatures, droplets evaporate more slowly and the temperature inside droplets has sufficient time to become almost homogeneous. Hence, the evaporation times predicted by the ETC and ITC models are close [23].

Fig. 3 illustrates the effect of a ETC model on the total ignition delay time at various initial gas temperatures in the presence of bag and stripping break-ups [23]. The initial droplet diameter and velocity are assumed equal to 50  $\mu$ m and 50 m/s respectively. Symbols in the figure indicate the values of initial gas temperatures for which calculations of the evaporation time were performed. The Shell model with  $A_{f4} = 3 \times 10^6$  was used. As can be seen from this figure, the ignition delay decreases with increasing  $T_g$ . The strong influence of the temperature gradient inside droplets on droplet break-up, evaporation and the ignition of evaporated fuel/air mixture, allowed the authors of [23] to recommend that this effect be taken into account in computational fluid dynamics codes designed to model fluid dynamics, heat transfer and combustion processes in internal combustion engines. So far this effect has been almost universally ignored, the only



**Figure 2.** The values of  $(R_d/R_{d0})^2$  for evaporating n-heptane droplets versus time for the initial pressure of 0.1 MPa, as measured by Nomura et al [59], and the results of calculations based on the ITC and the ETC models implemented into the zero-dimensional code. The values of the initial gas temperatures 471 K, 555 K, 647 K and 741 K are indicated near the plots. The effects of radiation were taken into account based on Equation (14) [23].



**Figure 3.** The plots of the total ignition delay versus  $T_g$  in the presence of the break-up for droplets with initial diameter and velocity equal to  $50 \mu\text{m}$  and  $50 \text{ m/s}$  respectively, calculated using the ITC and the ETC models implemented into the zero-dimensional code. Symbols indicate the values of gas temperature for which the ignition delay times were calculated [23].

exception, to the best of our knowledge, being paper [32].

To summarise the results reported in [23], in the absence of break-up the influence of temperature gradient on droplet evaporation in realistic diesel engine conditions was shown to be 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 effect of the temperature gradient inside droplets leads to a substantial increase in droplet surface temperature at the initial stages of its heating. This increase, in turn, leads to a decrease in droplet surface tension and a decrease in the threshold radii at which break-up occurs, 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 was shown to lead 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 is enhanced substantially, leading to more than the halving of the total ignition delay. This reduction of the total ignition delay time was understood to be due to the 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 be taken into account in CFD codes describing droplet break-up and evaporation processes, and the ignition of the evaporated fuel/ air mixture.

## **6. Heating, evaporation and ignition of fuel droplets: combined asymptotic and numerical analysis**

Although the numerical analysis of the problem of heating and evaporation of droplets and ignition of fuel vapour/air mixture based on Equations (1), (4), (6), (7) and (8) is widely used in engineering application, the difficulties and limitations of this analysis are well known. In realistic engineering application when thousands of droplet parcels can be calculated in each computational cell the number of equations solved could reach several thousands (and the number of computational cells can reach millions). Hence, the direct solution of this system using available ODEs solvers is not feasible. Following widely used practice in CFD codes, this system of equations is decomposed into subsystems which are solved sequentially. When each of these subsystems is solved, the remaining variables are assumed to have constant values over the time step. This approach is widely referred to as the operator splitting technique (see [61]). Following [21] this approach is called the ‘fixed decomposition approach’. One of the main problems with this approach is the choice of the time step over which the ODEs are solved. This choice would be easy if the characteristic time scales of all equations involved had the same order of magnitude. Unfortunately, in realistic applications this is practically never the case, and the system of ODEs under consideration is stiff. If, in this situation, we choose the time scale equal to the shortest time scale in the system, then we waste computer resources by calculation of equations where the values of variables remain practically constant over this time scale. If, however, a time scale longer than the shortest time scale is chosen then the accuracy of the calculations could be compromised.

Further discussion of this problem and ways to overcome it is based on the analysis reported in [21]. As noticed in [21], to overcome this problem the multi-scale nature of ODEs needs to be investigated before any attempt to solve them is made. This idea could be prompted by the approaches used in [62] for the analysis of the processes in CO<sub>2</sub> lasers and the one used in [63] for the analysis of equations describing the autoignition of diesel fuel (the Shell model). Before solving a system of five stiff ODEs describing five temperatures in these lasers, the characteristic time-scales of these equations were analysed [62]. It was shown that two of these equations describe rather rapid relaxation of two temperatures to the third one. This allowed the authors of [62] to replace the system of 5 stiff equations by a system of 3 non-stiff equations

without any significant loss of accuracy. The approach used in [63] was different from that used in [62]. However, both methods result in the reduction of the number of ODEs to be solved, and elimination of the stiffness of the system of equations. In mathematical terms, in both papers the dimension of the ODE system was reduced. In other words, the system was decomposed into lower dimension subsystems.

A similar system decomposition into lower dimension subsystems has been used in constructing reduced chemical mechanisms based on Intrinsic Low-Dimensional Manifolds (ILDM) (e.g. [64] - [66]) and Computational Singular Perturbation (CSP) (e.g. [67] - [71]). There are many similarities between these methods. They are based on a rigorous scale separation such that ‘fast’ and ‘slow’ subspaces of the chemical source term are defined and mechanisms of much reduced stiffness are constructed. These approaches, however, were developed with a view to modelling chemical kinetics. Their generalization to other problems has not been considered, to the best of our knowledge.

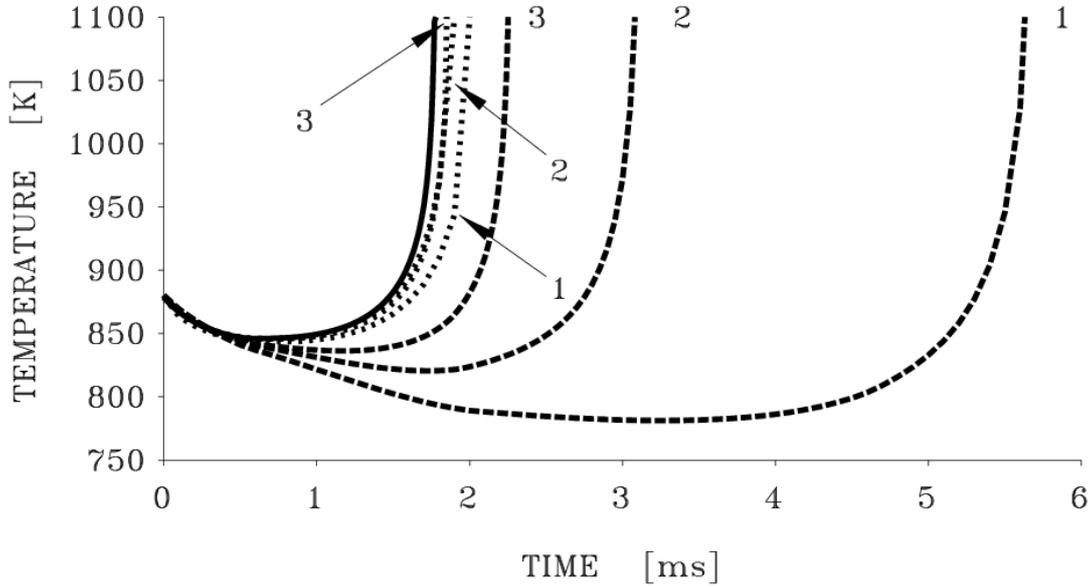
A useful analytical tool for the analysis of stiff systems of ODEs, used for the modelling of spray heating, evaporation and ignition, could be based on the geometrical asymptotic approach to singularly perturbed systems. Its application to the asymptotic analysis of the processes of heating and evaporation of fuel droplets and ignition of fuel vapour/ air mixture was discussed in Section 4.

These approaches to the decomposition of systems of ODEs were developed and investigated with a view to their application to rather special problems, and were based on a number of assumptions. These include fixing the decomposition over the whole period of the process, and not allowing its hierarchy to change with time. The underlying philosophy of these approaches, however, seems to have relevance to a wide range of physical and engineering problems including spray modelling in general CFD codes. The development of a fairly general new method of decomposition of a system of ODEs, allowing a change in the nature of the decomposition with time (dynamic decomposition), was the main objective of the research reported in [21].

As in the original integral manifold method, the formal approach to the decomposition of the system of ODEs used in [21] is based on the division of system variables into ‘fast’ and ‘slow’. This leads to the division of this system onto ‘fast’ and ‘slow’ subsystems. In contrast to the original version of the integral manifold method, however, linearised variations of slow variables during the time evolution of the fast variables were taken into account in the first order approximation to the fast manifold. The utility of this division depends on whether the ‘fast’ subsystem has a lower dimension than the ‘slow’ subsystem. The procedure can be iterative and result in a hierarchical division of the original system. For example the ‘slow’ subsystem can, in its turn, be subdivided into ‘slow’ and ‘very slow’ subsystems. The proposed procedure was initially focused on the simplest possible subdivision of the original system into two subsystems, and applied to spray combustion modelling. Note that ‘fast’ – ‘slow’ decompositions in this case could be different for different phase space regions and for different time intervals.

This new method was applied to simulate polydisperse spray heating, evaporation and ignition based on Equations (1), (4), (6), (7) and (8) [21]. The model was chosen to be simple, but capable nevertheless of capturing the essential features of the process. Three droplets with initial radii  $5\ \mu\text{m}$ ,  $9\ \mu\text{m}$  and  $13\ \mu\text{m}$  respectively were considered. The initial temperatures of all droplets was taken to be 400 K. The gas temperature was taken to be 880 K. The gas volume was chosen such that if the droplets were fully evaporated without combustion then the equivalence ratio of fuel vapour/air mixture was equal to 4. This is the situation typical of diesel engines in the vicinity of the nozzle. The initial density of oxygen was taken to be equal to  $2.73\ \text{kg/m}^3$  (this corresponds to air pressure equal to 3 MPa). The initial mass fraction of fuel was taken to be zero. These values of the parameters can be considered as an approximation to the actual conditions in diesel engines.

Once the smaller droplets had evaporated, the number of equations was reduced. These



**Figure 4.** Plots of gas temperature versus time, calculated using the first approach (fixed decomposition) (dashed), second approach (coupled solution of the full system of equations) (solid), and the third approach (dynamic decomposition) (dotted). Plots ‘1’, ‘2’ and ‘3’ refer to calculations based on the time steps  $10^{-4}$  s,  $5 \times 10^{-5}$  s and  $10^{-5}$  s respectively. The gas volume is chosen such that if the droplets are fully evaporated without combustion then the equivalence ratio of fuel vapour/air mixture is equal to 4 [21].

coupled equations were solved using three approaches [21]. Firstly, following a widely used practice in CFD codes, the system of equations was divided into subsystems which were solved sequentially. Secondly, these equations were solved rigorously using the DLSODAR stiff solver from ODEPACK developed in the Lawrence Livermore National Laboratory. This means that all equations were solved simultaneously. The third approach was based on decomposing the original system following the procedure described above.

The time evolution of gas temperature calculated using the three approaches, is shown in Fig. 4 [21]. As follows from Fig. 4, the first approach appears to be very sensitive to the time step. If the time step  $10^{-4}$  s was chosen then the predicted total ignition delay is almost four times longer than the one predicted based on the second approach (coupled solution of the whole system). If the time step is decreased to  $5 \times 10^{-5}$  s and  $10^{-5}$  s then calculations using the first method appear to be more accurate than in the case when this time step is equal to  $10^{-4}$  s, but still the accuracy of computations is hardly acceptable for practical applications. Even for a rather small time step,  $10^{-5}$  s, the predicted total ignition delay is more than 20% greater than predicted by the rigorous coupled solution of this system of equations (second approach). The application of the third approach to the solution of this system gives a rather different picture. Even in the case of the largest time step ( $10^{-4}$  s) the error in calculations of the total ignition time delay is just 13%. In the case of smaller time steps, the time delay predicted by solving the decomposed system almost coincides with the one obtained by rigorously solving the whole

system with possible errors not exceeding 2%. Essentially the same conclusion regarding the benefits of the third approach based on the decomposition of the original system of equations follows for other variables.

## 7. Conclusions

Recent progress in the development of a combined analytical, asymptotic and numerical approach to modelling of heating and evaporation of fuel droplets and ignition of fuel vapour/ air mixture has been discussed. This includes modelling of droplet heating and evaporation by convection and radiation from the surrounding hot gas based on a combined analytical and numerical approaches, as suggested in [19]. The finite thermal conductivity of droplets and recirculation in them were taken into account. These approaches are based on the incorporation of analytical solutions of the heat conduction equation inside the droplets (constant or almost constant convection heat transfer coefficient  $h$ ) or replacement of the numerical solution of this equation by the numerical solution of the integral equation (arbitrary  $h$ ). It was shown that the solution based on the assumption of constant  $h$  is most computer efficient for implementation into numerical codes. This solution was applied to the first time step, using the initial distribution of temperature inside the droplet. The results of the analytical solution over this time step were used as the initial condition for the second time step etc. This approach was applied to conditions relevant to diesel engines. It was shown to be more effective than approaches based on the numerical solution of the discretised heat conduction equation inside the droplet, and more accurate than solutions based on the parabolic temperature profile model. It was shown that the contribution of thermal radiation to droplet heating and evaporation could be taken into account using a simplified model, which does not consider the variation of radiation absorption inside droplets [19, 20, 25].

The results of the analysis of the simplified problem of heating and evaporation of diesel fuel droplets and ignition of fuel vapour/ air mixture based on the asymptotic method of integral manifolds have been discussed based on [24]. The semi-transparency of droplets was taken into account, and a simplified model for droplet heat-up was used. The results were applied to the modelling of thermal explosion in diesel engines. Two distinct dynamical situations were considered, depending on the initial parameters. These are ‘far zone’ (small initial liquid volume fraction and small droplet radii) and ‘near zone’ (large initial liquid volume fraction and large droplet radii). The conditions of the first zone are typical for the areas in the combustion chamber which are far from the fuel injectors, while the conditions of the second zone are typical for the areas in the combustion chamber which are relatively close to the fuel injectors. It was pointed out that small droplet heating and evaporation time in the far zone is smaller than the chemical ignition delay of the fuel vapor/air mixture. The total ignition delay decreased with increasing initial gas temperature. In the near zone for large droplets, the process was shown to start with the initial gas cooling and slight heating of droplets. This was followed by a relatively slow heating of gas due to the chemical reaction, and further droplet heating. The total ignition delay in the near zone was shown to be larger than in the far zone. It was expected that before thermal explosion in the near zone takes place, the droplets break-up and are removed from this zone.

The results of investigation of the effect of the temperature gradient inside fuel droplets on droplet evaporation, break-up and the ignition of fuel vapour/ air mixture based on a new zero-dimensional code are reviewed based on [23]. This code takes into account the coupling between the liquid and gas phases and describes the autoignition process based on the eight step chain branching reaction scheme (the Shell model). The effect of temperature gradient inside droplets was investigated by comparing the ‘effective thermal conductivity’ model and the ‘infinite thermal conductivity’ model, both of which have been implemented in this code. The predictions of the code were validated against available experimental data. It was pointed

out that in the absence of break-up, the influence of the temperature gradient in droplets on droplet evaporation in a realistic diesel engine environment is generally small. In the presence of the break-up process, however, the temperature gradient inside the droplets can lead to a significant decrease in evaporation time. Even in the absence of break-up, the effect of the temperature gradient inside the droplets was shown to lead to a noticeable decrease in the total ignition delay. In the presence of break-up this effect was shown to be substantially enhanced. It was recommended that the effect of the temperature gradient inside the droplets is taken into account in CFD codes describing droplet break-up and evaporation processes, and the ignition of the evaporated fuel/ air mixture [23].

A new decomposition technique for a system of ODEs, based on the geometrical version of the integral manifold method has been discussed based on [21]. This was based on comparing the values of the right hand sides of ODEs, leading to the separation of the equations into ‘fast’ and ‘slow’ variables. The hierarchy of the decomposition was allowed to vary with time. Equations for fast variables were solved by a stiff ODE system solver with the slow variables taken at the beginning of the time step. The solution of the equations for the slow variables was presented in a simplified form, assuming a linearised variation of these variables for the known time evolution of the fast variables. This can be considered as the first order approximation for the fast manifold. 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 [21].

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