Multiple scales in spray modelling

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Abstract. A summary of the results of modelling of several processes in diesel engine sprays is presented. These include spray penetration, droplet heating and droplet evaporation. Typical scales of these processes differ by more than 7 orders of magnitude from about $3 \times 10^{-2}$ m (spray penetration) to about $10^{-9}$ m (diameters of individual molecules). It has been confirmed that the dynamic decomposition techniques for solving stiff systems of ordinary differential equations, reported earlier, can be an effective tool in spray modelling applications for CFD codes.

1. Introduction

The problem of spray modelling have been discussed in numerous monographs and review papers (e.g. [1]-[9]). A number of reviews have been focused on various specific aspects of this modelling, including heating and evaporation of individual droplets [10, 11]. The main objective of this paper is to present an overview of the results, not covered in the previous paper [11] with particular emphasis on the multiscale nature of the models.

A spray can be defined as one of the types of two phase flow, involving liquid as the dispersed phase in the form of droplets or ligaments and a gas as the continuous phase (cf. the definition given in [1]). In the environment, sprays are easily observed; rain, waterfalls and volcanic eruptions are just a few examples. They are widely used in medical and engineering applications, including those in direct injection internal combustion engines. This paper will focus mainly on the latter, although the generalisation of the results to other types of sprays is straightforward.

Modelling of sprays involves analysis of a number of processes which can take place simultaneously. These processes include spray formation, break-up of the liquid jet, ligaments and individual droplets, cavitation inside the nozzle, droplet heating and evaporation and, in the case of internal combustion engines, ignition of the fuel vapour/air mixture. These processes take place over vastly different scales in space and time. For example, a typical spray penetration length in diesel engines used in passenger cars is $3 \times 10^{-2}$ m. The diameter of the nozzle in these engines is about $10^{-4}$ m; a typical droplet diameter is about $10^{-5}$ m. The thickness of the Knudsen layer around droplets is about $10^{-7}$ m, while the diameter of individual molecules is about $10^{-9}$ m.

This review will focus on: modelling spray penetration, when the effect of droplet heating and evaporation can be ignored (Section 2); modelling of the heating of individual droplets when the effects of evaporation can be ignored (Section 3); and the modelling of droplet evaporation (Section 4). In Section 5 some results of further developments of the dynamic decomposition technique, already discussed in [11], are summarised.
2. Spray penetration

Detailed comparisons between different models for spray penetration and experimental results were given by Dent [12] and Hay and Jones [13]. They concluded that models predicting the penetration distance $s$ to be proportional to the square root of time $\sqrt{t}$ are in good agreement with observations. This was confirmed by Sendyka [14]. A more detailed analysis of the penetration length shows that the proportionality of $s$ to $\sqrt{t}$ only occurs at times exceeding the so called jet break-up time. At shorter times, $s$ is proportional to $t$ [15]. There is some ambiguity, however, regarding the definition of the jet break-up time.

The problem of modelling spray penetration is closely linked to the problem of modelling induced air velocity within droplet driven sprays. The latter was studied by Ghosh and Hunt [17], and some of their results were incorporated into the spray penetration model described in [16]. In [17] 3 spray zones were considered: zone 1, where the initial velocities of droplets are much greater than that of the air stream and are not much affected by it; zone 2, where the droplets slow down and their velocities become comparable with the air velocity; zone 3, where the droplets’ velocities decrease so much that they becomes less than the terminal velocity. These zones, introduced in [17], have the same physical meanings as mixing, transition and fully developed regions considered in [15].

Firstly, the focus of this section will be on the analysis of a simple model referring to zone 3, which was suggested in [16], and its possible further developments. Secondly, a simplified model referring to zone 1, developed in [16, 18], will be considered.

2.1. Two-phase flow

When the distance from the nozzle becomes large enough, the velocity of the entrained air approaches the velocity of droplets. As a result, the dynamics of both droplets and entrained air can be described in terms of a two phase flow with a zero relative velocity between air and droplets. The basic properties of this flow can be derived from the equations of conservation of mass and momentum.

From the equation of conservation of mass of droplets we obtain [16]:

$$\rho_l A_0 v_{in} = \rho_m A_m v_m - (1 - \alpha_d) A_m \rho_g v_m,$$  

(1)

where $A_0$ is the cross-sectional area of the nozzle, $v_{in}$ is the initial velocity of droplets, $\rho_l$ is the density of liquid (droplets), $\rho_m$ is the density of a mixture of droplets and gas, $A_m$ is the cross-sectional area of a spray, $v_m$ is the velocity of a mixture, $\alpha_d$ is the volume fraction of droplets. The left hand side of Equation (1) is the mass flow rate of fuel at the nozzle. The second term in the right hand side of Equation (1) takes into account the contribution of the mass flow rate of entrained air. The first term in the right hand side of this equation gives the mass flow rate of the mixture of fuel and air. The relation between $A_m$ and $A_0$ can be presented in the form [16]:

$$A_m = A_0 + \pi D_0 s \tan \theta + \pi s^2 \tan^2 \theta,$$  

(2)

where $\theta$ is the half angle of the spray cone.

Equation (1) should be supplemented by the equation of conservation of momentum:

$$\rho_l A_0 v_{in}^2 = \rho_m A_m v_m^2,$$  

(3)

The combination of Equations (1) – (3) leads us to the following equation for the velocity of spray penetration [16]:

$$\frac{ds}{dt} |_m = \frac{2v_{in}}{1 + \sqrt{a + bs + cs^2}},$$  

(4)
Thus:

\[ a = 1 + 4(1 - \alpha_d)\tilde{\rho}_a; \quad b = \frac{16(1 - \alpha_d)\tilde{\rho}_a\tan \theta}{D_0}; \quad c = \frac{16(1 - \alpha_d)\tilde{\rho}_a\tan^2 \theta}{D_0^2}, \]

\[ \tilde{A} = A_m/A_0 = 1 + \frac{4s\tan \theta}{D_0} + \frac{4s^2\tan^2 \theta}{D_0^2}; \quad \tilde{\rho}_r = \rho_m/\rho_l; \quad \tilde{\rho}_a = \rho_g/\rho_l; \quad \tilde{v} = v_{in}/v_m. \]

Subscript \( m \) indicates that \( \frac{ds}{dt}|_m \) is the velocity of the mixture.

As follows from (4), in the case of no entrained air (\( \alpha_d = 1 \)) we have \( \tilde{v} = 1 \), which means that \( v_m = v_{in} \). This solution, however, does not have a physical meaning since the formation of spray always includes the entrained air. In a realistic spray environment \( \alpha_d \ll 1 \).

Integration of (4) gives [16]:

\[ s + 2cs + \frac{b}{4c}\sqrt{a + bs + cs^2} - \frac{b\sqrt{a}}{4c} + \frac{4ac - b^2}{8c^{3/2}}\ln \left[ \frac{2\sqrt{c(a + bs + cs^2) + 2cs + b}}{2\sqrt{ac + b}} \right] = 2v_{in}t. \tag{5} \]

In the case when \( a \gg bs \gg cs^2 \) (the immediate vicinity of the nozzle), Equation (5) is simplified to [16]:

\[ s = \frac{2v_{in}t}{1 + \sqrt{a + \frac{b}{8c\sqrt{a}}(a - 1)}} \approx v_{in}t. \tag{6} \]

When deriving (6) the fact that \( \tilde{\rho}_a \ll 1 \) and \( a - 1 \ll 1 \) is taken into account. If \( a \ll bs \ll cs^2 \) (\( s \) is large and/or \( D_0 \) is small) then \( \frac{b}{2\sqrt{ac}} \approx 2\sqrt{\tilde{\rho}_a} \ll 1 \) and the logarithmic term can be ignored. Thus:

\[ s = \frac{\sqrt{v_{in}D_0}t}{(1 - \alpha_d)^{1/4}\tilde{\rho}_a^{1/4}\sqrt{\tan \theta}} \left( 1 - \frac{\sqrt{D_0}}{4\sqrt{v_{in}(1 - \alpha_d)^{1/4}\tilde{\rho}_a^{1/4}\sqrt{\tan \theta}}\sqrt{t}} \right). \tag{7} \]

Equation (7) can be further simplified if the second term in the right hand side is ignored:

\[ s = \frac{\sqrt{v_{in}D_0}t}{(1 - \alpha_d)^{1/4}\tilde{\rho}_a^{1/4}\sqrt{\tan \theta}}. \tag{8} \]

Equation (8) is identical to the one suggested by a number of authors (see [12]). Equations (7) and (6) can be considered as generalisations of previously discussed formulae. The combination of Equations (6) and (8) gives essentially the same expression for spray penetration as discussed in [2]. The main advantage of Equation (5) is that it can accurately predict a smooth transition from the immediate vicinity of the nozzle to the two-phase flow in the region where the spray is fully formed. Separate solutions for the near zone and the far zone, discussed in [15], inevitably lead to a physically unrealistic jump in the velocity between these zones. The range of applicability and accuracy of Equation (8) can be determined based on direct comparison between the predictions of Equations (5), (6) and (7) and the available experimental data. In [19] the predictions of the above mentioned equations were compared with the results of experimental studies of spray penetration, obtained using a rapid compression diesel spray rig based at Brighton University (UK) and a high-pressure dimethyl ether spray chamber based at Chungbuk National University (Korea). In both cases the experimental results are shown to be in agreement with the prediction of theoretical models, even though the equipment used and the range of ambient densities tested varied significantly between the two studies. In most cases, however, the errors of measurement seem to be comparable with the improved accuracy offered by Eq. (7). The model suggested in [16] is based on the assumption that the effects of turbulence on spray dynamics can be ignored. The latter effects lead to spray diffusion in
directions perpendicular to the spray penetration. Taking into account this effect leads to a
new spray penetration model which predicts that $s \propto t^{3/2}$\footnote{20}. Although this dependence has
occasionally been observed in our experiments, it cannot be considered as typical.

More advanced models of spray penetration, based on mass and momentum conservation,
but taking into account the non-zero velocity between droplets and gas, have been developed in
numerous papers including \footnote{21}-\footnote{23}. In this case the effect of droplet evaporation also needs to be
taken into account. In gasoline sprays, the spray penetration process is sometimes accompanied
by the formation of vortex rings \footnote{24}. In this case a different approach to the analysis would be
required (cf. \footnote{24}).

The overall spray penetration length, discussed so far, is the largest measure used for the
analysis of sprays. In the next section the focus will be on the initial stage of spray penetration.

2.2. The initial stage

In this section, the results reported earlier in \footnote{16, 18} are briefly summarised. The contribution
of the jet in the spray penetration process can be ignored as the first approximation, and the
initial sizes of droplets can be assumed equal to the nozzle diameter \footnote{16}. This can be justified
by the fact that for typical diesel engines the expected break-up regime lies between the first
and second wind induced break-ups \footnote{25}.

At the initial stage of spray penetration the analysis can be focused on the equation describing
the dynamics of an individual droplet:

$$\frac{d^2s}{dt^2} = -\frac{3}{8R_d} \frac{C_D \rho_g}{\rho_l} \left( \frac{ds}{dt} - v_g \right) \left| \frac{ds}{dt} - v_g \right|,$$

\begin{equation} \tag{9} \end{equation}

where $C_D$ is the drag coefficient, which depends on the Reynolds number $Re = 2\rho_g|v_d-v_g|R_d/\mu_g$.
$R_d$ is the droplet’s radius, $v_d = \frac{ds}{dt}$, $v_g$ is the gas velocity, and the droplet is assumed to be a
perfect sphere.

Equation (9) refers to the smallest scale considered so far which is comparable with the
diameter of the nozzle. The solution of this equation requires knowledge of $C_D$ and $v_g$. A number
of approximations for $C_D$ have been suggested (\footnote{15}, \footnote{26}-\footnote{30}). The one given in \footnote{31} was used
in our analysis. In this approximation, three ranges of Reynolds numbers were considered: $Re \leq 2$ (Stokes flow), $2 < Re \leq 500$ (Allen flow) and $500 < Re \leq 10^5$ (Newton flow). The functions
$C_D(Re)$ for these flows are given by the following expressions: $C_D = 24/Re$ (Stokes flow),
$C_D = 18.5/Re^{0.8}$ (Allen flow) $C_D = 0.44$ (Newton flow). The condition $Re < 10^5$ is always
satisfied for realistic droplets in diesel engines. Note that there is a printing mistake in \footnote{31}
referring to the value of Re when the transition from Stokes to Allen flow takes place. This
mistake was overlooked in the original paper \footnote{18}.

The drag force acting on the droplets leads not only to their deceleration, but also to
momentum transfer from the droplets to the gas entrained into the spray. In \footnote{17} the following
equation for gas velocity in zone 1 of the spray was derived:

$$\frac{d}{ds} \left( \pi R_j^2 v_g^2 \right) = \frac{3\pi R_s^2 \alpha_d}{8R_d} C_D (v_d - v_g)^2,$$

\begin{equation} \tag{10} \end{equation}

where $R_j$ and $R_s$ are radii of the gas/air jet and the spray itself respectively at a certain position
$s$, $R_j$ is usually slightly larger than $R_s$, but as a first approximation we will assume that they
are both equal to $s \tan \theta$.

We assume that $v_g$ is so small compared with $v_d$ that its contribution in the right hand side
of Eq. (9) can be ignored altogether. Remembering the definitions of $C_D$ for the three types of
flow, Equation (9) can be simplified to \footnote{18}:

$$\frac{d^2s}{dt^2} = -\frac{9}{2} \frac{\mu_g}{\rho_l R_j^2} \frac{ds}{dt} \quad \text{(Stokes flow)},$$

\begin{equation} \tag{11} \end{equation}
\[ \frac{d^2 s}{dt^2} = -\frac{4.577 \mu_v^{0.6} \rho_g^{0.4}}{\rho_l R_d^{1.6}} \left( \frac{ds}{dt} \right)^{1.4} \] (Allen flow),

\[ \frac{d^2 s}{dt^2} = -\frac{0.165 \rho_g}{\rho_l \gamma} \left( \frac{ds}{dt} \right)^2 \] (Newton flow).

Assuming that \( R_d = \text{const} \) (no evaporation and break-up) the solutions of Equations (11) – (13) can easily be found [16]. The effect of air entrainment can be considered as the perturbation to the solutions of Equations (11) - (13) [16]. This leads us to the following expressions for \( s \) in the limit of small \( t \):

\[ s = v_d t - \frac{1}{2} v_d t^2 + 4 \frac{\alpha_s \sqrt{v_d t}}{15} \] (Stokes flow),

\[ s = v_d t - 0.5 v_d t^2 + 0.373 \kappa e v_d^0 \beta t^{5/2} \] (Allen flow),

\[ s = v_d t - 0.5 v_d^2 \gamma t^2 + 0.533 \gamma v_d^3 t^{5/2} \] (Newton flow),

where \( v_d \) is the initial droplet velocity,

\[ \kappa_e = \frac{3 R_d^2 \alpha_s}{8 R_d^2 \rho_i C_D v_d^2}, \quad \alpha_s = \frac{9 \nu_g \rho_g}{2 R_d^2 \rho_i}, \quad \beta = \frac{4.577 \nu_g}{R_d^{1.6} \rho_i}, \quad \gamma = \frac{0.165 \rho_g}{R_d \rho_i}. \]

The main novelty of Equations (14)-(16) is the contribution of the terms taking into account air entrainment (terms proportional to \( t^{5/2} \)). The main limitation of these equations is that they do not consider the contribution of droplet break-up. Among numerous droplet break-up models suggested so far we mention the bag and stripping break-up models [32, 33], WAVE break-up model [34], Taylor Analogy Break-up (TAB) model [35] and the stochastic break-up model developed in [36, 37]. The bag and stripping break-up models turned out to be particularly important for the analytical study of the effects of break-up on spray penetration. They were used in [16, 18]. Other models have been used in numerical simulations of spray dynamics [38, 37]. The analysis of these models and their implementation into computational fluid dynamics codes is beyond the scope of this paper.

Also this approach does not take into account the effects at scales less that the diameter of the nozzle in the immediate vicinity of the nozzle. The most important of these effects is cavitation inside the nozzle [39, 40].

The scales considered so far refer mainly to the range from about \( 10^{-4} \text{ m} \) (typical diameter of the nozzle) to about \( 10^{-2} - 10^{-1} \text{ m} \) (typical penetration length). In the following section we move to scales of about \( 10^{-5} \text{ m} \) (typical diameter of droplets away from the nozzle).

3. Droplet heating

The problem of the transient heating of semitransparent spherical droplets immersed in a stationary hot gas, taking into account the effect of thermal radiation, has been considered by a number of authors (see e.g. [41]-[45]). One of the main assumptions made in all these papers is that the boundary layer around droplets has developed and steady state correlations for the convection heat transfer coefficient (Nusselt number) can be used. A brief review of some of the results reported in these papers is given in [11].

In the general case, the process of droplet heating takes place simultaneously with the formation of the boundary layer. For moving droplets this is a complicated problem, requiring a numerical solution. The heating of stagnant droplets by the ambient gas reduces to a conduction...
problem. Assuming the spherical symmetry of the problem, its mathematical formulation is based on the solution of the equation:

\[
\frac{\partial T}{\partial t} = \kappa \left( \frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right) + P(R, t),
\]

where

\[
\kappa = \begin{cases} 
\kappa_l = \frac{k_l}{(c_l\rho_l)} & \text{when } R \leq R_d \\
\kappa_g = \frac{k_g}{(c_g\rho_g)} & \text{when } R_d < R \leq \infty,
\end{cases}
\]

\(\kappa_l, \kappa_g\) and \(c_l, c_g\) are the liquid (gas) thermal diffusivity, thermal conductivity and specific heat capacity respectively, \(R\) is the distance from the centre of the sphere.

This equation needs to be solved subject to the following initial and boundary conditions:

\[
T|_{t=0} = \begin{cases} 
T_{d0}(R) & \text{when } R \leq R_d \\
T_{g0}(R) & \text{when } R_d < R \leq R_g,
\end{cases}
\]

\[
T|_{R=R_d} = T|_{R=R_d+0} = \begin{cases} 
\kappa_l \frac{\partial T}{\partial R} |_{R=R_d} & = k_g \frac{\partial T}{\partial R} \big|_{R=R_d+0} & ; \quad T|_{R_g} = T_{g0}.
\end{cases}
\]

Assuming that \(T_{d0}(R) = T_{d0} = \text{const}_1\) and \(T_{g0}(R) = T_{g0} = \text{const}_2, R_g = \infty, \) and ignoring the effect of thermal radiation, Cooper [46] has solved this problem analytically:

\[
T(R \leq R_d) = T_{g\infty} + \frac{2k_l}{\pi k_g} \sqrt{\frac{\kappa_g}{\kappa_l}} (T_{g\infty} - T_{d0}) \frac{R_d}{R} \int_0^\infty du \Phi(u) \exp \left( -u^2 \text{Fo} \frac{\kappa_l}{\kappa_g} \right) \sin \left( u \frac{R}{R_d} \right),
\]

\[
T(R \geq R_d) = T_{g\infty} + \frac{2k_l}{\pi k_g} \sqrt{\frac{\kappa_g}{\kappa_l}} (T_{g\infty} - T_{d0}) \frac{R_d}{R} \int_0^\infty \frac{du}{u} \Phi(u) \exp \left( -u^2 \text{Fo} \frac{\kappa_l}{\kappa_g} \right) \times \left\{ \cos(\gamma_c u) \sin u + \sqrt{\frac{\kappa_g}{\kappa_l}} \sin \gamma_c \left[ \frac{k_l}{k_g} (u \cos u - \sin u) + \sin u \right] \right\},
\]

where

\[
\Phi(u) = \frac{(u \cos u - \sin u)}{u^2 \sin^2 u + \frac{\kappa_g}{\kappa_l} \left[ k_l (u \cos u - \sin u) + \sin u \right]^2},
\]

\[
\text{Fo} = \frac{t \kappa_g R_d^2}{R^2} \quad (\text{Fourier number}),
\]

\[
\gamma_c = \sqrt{\frac{\kappa_l}{\kappa_g}} \left[ \frac{R - R_d}{R} \right] u.
\]

As expected, this solution predicts diffusion of heat from gas to droplets, if \(T_{g\infty} > T_{d0}\). Initially, the heat flux from gas to droplets predicted by the equation

\[
\dot{q} = -k_g \frac{\partial T}{\partial R} \big|_{R=R_d+0}
\]

is infinitely large. It approaches zero at \(t \to \infty\).
An alternative solution of Equation (17), taking into account the absorption of thermal radiation inside the droplet, finite \( R_g \) and the dependence of \( T_{g0} \) on \( R \) was suggested in [47, 48]:

\[
T(R, t) = T_{g0} + \frac{1}{R} \sum_{n=1}^{\infty} \left[ \exp \left( -\lambda_n^2 t \right) \frac{1}{||v_n||^2} \int_0^{R_d} \left( -T_{g0} - T_{d0}(R) \right) \rho c v_n(R) c_1 \rho_l dR \right. \\
+ \left. \int_0^t \exp \left( -\lambda_n^2 (t - \tau) \right) p_n(\tau) d\tau \right] v_n(R),
\]

(24)

where

\[
v_n(R) = \begin{cases} \\
sin(\lambda_n a_d R) & \text{when } R < R_d \\
sin(\lambda_n a_d (R - R_g)) & \text{when } R_d \leq R \leq R_g,
\end{cases}
\]

(25)

\[
||v_n||^2 = \frac{c_1 \rho_l R_d}{2 \sin^2(\lambda_n a_d R_d)} + \frac{c_{pg} \rho_g (R_g - R_d)}{2 \sin^2(\lambda_n a_g (R_d - R_g))} - \frac{k_l - k_g}{2 R_d \lambda_n^2},
\]

\[
p_n(t) = \frac{c_1 \rho_l}{||v_n||^2} \int_0^{R_0} R P(t, R) v_n(R) dR.
\]

A countable set of positive eigenvalues \( \lambda_n \) is found from the solution of the equation:

\[
\sqrt{k_l c_1 \rho_l \cot(\lambda_a R_b)} - \sqrt{k_g c_{pg} \rho_g \cot(\lambda_a (R_d - R_g))} = \frac{k_l - k_g}{R_d \lambda^n}.
\]

(26)

These are arranged in ascending order \( 0 < \lambda_1 < \lambda_2 < \ldots \) \( a_d = \sqrt{\frac{c_{pg} \rho_g}{k_t}}, a_g = \sqrt{\frac{c_{pg} \rho_g}{k_g}} \).

The practical implementation of any of these solutions into computational fluid dynamics codes remains unclear, since these codes are based on the separation of the processes in the liquid and gas phases. The required separation between the solutions could be achieved based on the comparison between the thermal diffusivities of gas and liquid. Following [10], let us consider typical values of parameters for diesel fuel spray droplets and assume that these droplets have initial temperature 300 K and are injected into a gas at temperature 800 K and pressure 30 atm [49]:

\[
\rho_l = 600 \text{ kg/m}^3, \quad k_l = 0.145 \text{ W/(mK)}, \quad c_l = 2830 \text{ J/(kgK)},
\]

\[
\rho_g = 23.8 \text{ kg/m}^3, \quad k_g = 0.061 \text{ W/(mK)}, \quad c_{pg} = 1120 \text{ J/(kgK)}.
\]

For these parameter values we obtain \( \kappa_l = 8.53 \times 10^{-8} \text{ m}^2/\text{s} \) and \( \kappa_g = 2.28 \times 10^{-6} \text{ m}^2/\text{s} \). This allows us to assume:

\[
\kappa_l \ll \kappa_g.
\]

(27)

This condition tells us that gas responds much more quickly to changes in the thermal environment than liquid. As a zeroth approximation we can ignore the changes in liquid temperature altogether, and assume that the droplet surface temperature remains constant in time. This immediately allows us to decouple the solution of Equation (17) from the trivial solution of this equation for the liquid phase \( T(R \leq R_d) = \text{const} \). The former solution can be presented as:

\[
T(R > R_d) = T_{g\infty} + \frac{R_d}{R} \left( T_{d0} - T_{g\infty} \right) \left[ 1 - \text{erf} \left( \frac{R - R_d}{2 \sqrt{\kappa_g t}} \right) \right],
\]

(28)

where

\[
\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt.
\]
In the limit \( R = R_d \), Equation (28) gives \( T = T_{d0} \). In the limit \( t \to 0 \), but \( R \neq R_d \), this equation gives \( T = T_{g\infty} \). From (28) we obtain the following equation for the heat flux from gas to droplets [50]:

\[
\dot{q} = \frac{k_g (T_{d0} - T_{g\infty})}{R_d} \left( 1 + \frac{R_d}{\sqrt{\pi \kappa_g t}} \right).
\]  

(29)

(cf. [51, 52]). For \( t \gg t_d \equiv R_d^2 / (\pi \kappa_g) \), Equation (29) can be further simplified to:

\[
|\dot{q}| = h (T_{g\infty} - T_{d0}),
\]  

(30)

where \( h = \frac{k_g}{R_d} \) is the convection heat transfer coefficient. Remembering the definition of the Nusselt number \( \mathrm{Nu} = 2 R_d h / k_g \), this value of \( h \) corresponds to \( \mathrm{Nu} = 2 \).

The equation similar to (30) could be obtained from Solutions (21) and (24) if we replace \( h \) in it with \( \tilde{h} = \frac{k_g}{R_d} \chi_t \), where in the case of Solution (21) the correction factor \( \chi_t \) is defined as [48]:

\[
\chi_t = \frac{\frac{1}{k_g} \int_0^\infty (u \cos u - \sin u) \Phi(u) \exp(-u^2 Fo \frac{\kappa_l}{\kappa_g}) du}{\int_0^\infty \sin u \Phi(u) \exp(-u^2 Fo \frac{\kappa_l}{\kappa_g}) du},
\]  

(31)

\( \Phi(u) \) is the same as in Equations (21) and (22).

In the case of Solution (24), \( \chi_t \) is defined as [48]:

\[
\chi_t = 1 + \frac{\Delta T_c + \Delta T_r}{T_{g0} - T_s},
\]  

(32)

where

\[
\Delta T_c = (T_{g0} - T_{d0}) k_l a_d a_g \sum_{n=1}^{\infty} A_n \exp(-\lambda_n^2 t),
\]  

(33)

\[
\Delta T_r = -3a \sigma R_d^{b-1} \frac{\theta_R^4 a_d}{a_g} \sum_{n=1}^{\infty} \frac{A_n}{\lambda_n^2} \left( 1 - \exp(-\lambda_n^2 t) \right),
\]  

(34)

\[
A_n = \frac{1}{||v_n||^2} \left[ R_d \cot(\lambda_n a_d R_d) - \frac{1}{\lambda_n a_d} \right] \cot(\lambda_n a_g (R_d - R_g)).
\]

When deriving Equation (34) the radiation term was presented in an explicit form [48]:

\[
P(R) = 3a \sigma R_d^{b-1} \frac{\theta_R^4}{c_l \rho_l},
\]  

(35)

where \( \theta_R \) is the radiation temperature,

\[
a = a_0 + a_1 \theta_R / 10^3 + a_2 \left( \theta_R / 10^3 \right)^2,
\]

\[
b = b_0 + b_1 \theta_R / 10^3 + b_2 \left( \theta_R / 10^3 \right)^2.
\]

\( \theta_R \) can be assumed equal to the external temperature in the case of an optically thin gas in the whole domain.

It was shown in [47, 48] that for \( R_g \geq 25 R_d \), the values of \( \chi_t \) defined by Eqs. (31) and (32) coincide for \( 0.1 \leq Fo \leq 100 \). In both cases they decrease from about 2.8 at \( Fo = 0.1 \) to about 0.6 at \( Fo = 100 \). It remains unclear how the multiscale nature of the processes in gas and liquid phases can be taken into account or described by the above mentioned solutions for temperature and heat fluxes.
4. Droplet evaporation

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 in the vicinity of the droplet surface is maintained at saturation level [10]. The applicability of this assumption to the problem of modelling droplet evaporation into a high pressure (above 1 atm) gas is not at first evident. Rigorous analysis of the dynamics of vapour molecules in the immediate vicinity of the droplets should be based on the analysis of the distribution function of background gas (air) \( f_\alpha \equiv f_\alpha(\mathbf{r}, t, \mathbf{v}) \) and vapour \( f_v \equiv f_v(\mathbf{r}, t, \mathbf{v}) \) using the Boltzmann kinetic equations. The general form of these equations, taking into account the interaction of vapour molecules with the background gas (air) can be presented as [53]:

\[
\frac{\partial f_\alpha}{\partial \mathbf{r}} + \mathbf{v}_a \frac{\partial f_\alpha}{\partial \mathbf{v}} = J_{aa} + J_{av} \]

\[
\frac{\partial f_v}{\partial \mathbf{r}} + \mathbf{v}_v \frac{\partial f_v}{\partial \mathbf{v}} = J_{va} + J_{vv} \]

(36)

where \( J_{\alpha\beta} (\alpha = a, v; \beta = a, v) \) are collision integrals defined as:

\[
J_{\alpha\beta} = \frac{\sigma_{\alpha\beta}^2}{\pi} \int_{-\infty}^{+\infty} \mathbf{v}_1 \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( f'_a f_{\beta 1} - f_a f'_{\beta 1} \right) |\mathbf{v}_a - \mathbf{v}_{\beta 1}| ,
\]

(37)

\( \sigma_{\alpha\beta} = (\sigma_\alpha + \sigma_\beta)/2 \), \( \sigma_\alpha \) and \( \sigma_\beta \) are the corresponding diameters of molecules, \( \theta \) and \( \phi \) are angular coordinates of molecules \( \beta \) relative to molecules \( \alpha \) after the collision, superscript \( ' \) indicates the velocities and the distribution functions after collisions. Subscript \( 1 \) indicates that molecules of type \( \beta \) collide with molecules of type \( \alpha \) and as a result of this interaction the function \( f_\alpha \) is modified. When deriving (36) and (37) it was assumed that molecules are rigid elastic spheres and body forces acting on them are negligible. These equations are solved subject to appropriate boundary and initial conditions, including the conditions at the droplet surface [53].

In the case of evaporation into a high pressure gas, Equations (36) are solved in a relatively thin layer in the immediate vicinity of the droplet surface (Knudsen layer). In the case of fuel droplet evaporation into a diesel engine combustion chamber with air pressure at about 30 atm, the thickness of this layer is less than \( 10^{-6} \) m [53]. This is a new scale of the problem. The solution of Equations (36) within this layer is performed at even smaller scales comparable with the diameter of individual molecules (about \( 10^{-9} \) m). This is the smallest scale of the problem.

The solutions of Equations (36) are matched with the solutions of the hydrodynamic equations at the outer boundary of the Knudsen layer. Since Equation (36) predicts the finite rate of detachment of vapour molecules from the surface of the droplet (in contrast to the infinite rate of this detachment predicted by the hydrodynamic models), the evaporation rate predicted by hydrodynamic models is always larger when compared with the rate predicted by kinetic models. Although the kinetic processes take place in a thin Knudsen layer, a noticeable reduction in the density of vapour is observed between the surface of the droplet and the outer boundary of this layer. In this case, the flux density of vapour, as predicted by the kinetic model, is controlled by the vapour density at the outer boundary of the Knudsen layer. The latter is less than the vapour density at the droplet surface, which controls the vapour flux predicted by the hydrodynamic model. This is consistent with the above mentioned conclusion regarding the evaporation rates predicted by kinetic and hydrodynamic models.

The solution of Equation (36) can be based on numerical methods only [53]. Asymptotic analysis of these equations is possible in some limiting cases. The analysis in [54] is based on the method previously reported in [55] and a number of simplified assumptions including ignoring the contribution of background gas in the Knudsen layer. Both rigorous numerical and asymptotic analyses led to essentially the same conclusions; even in the case of fuel droplet evaporation into a very high pressure gas (30 atm; the situation typical for diesel engines), the kinetic effects can lead to a noticeable reduction in droplet evaporation time (about 5-10 % for droplets with radii 5-10 \( \mu \)m).
5. Coupled solutions
Although the processes considered so far have scales which differ by more than 7 orders of magnitude, this does not bring any additional complexity to their analysis. This is related to the fact that the rate of change of these scales with time is generally small, and the hierarchy of scales remains unchanged. This, however, is not always the case, especially when chemical reactions (autoignition) become involved. This leads us to the problem of dynamic decomposition of the system of ordinary differential equations describing the processes in individual computational cells [56]. A summary of the main results of the latter paper was reported in [11]. This approach is based on comparing the values of the right hand sides of the equations, leading to the separation of the equations into ‘fast’ and ‘slow’ variables. The hierarchy of the decomposition is allowed to vary with time. Equations for fast variables are 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 is presented in a simplified form, assuming 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 is 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 system of equations and the solution of the decomposed system of equations was shown to be negligibly small for practical applications.

The model described in [56] has been further developed in [57, 58]. In [57], the description of the autoignition process based on the one-step Arrhenius reaction was replaced by its description in terms of the so called Shell model [59]-[62]. The main conclusions of this paper were essentially the same as those of [56]. In [58], a new approach to dynamic decomposition of the systems of ODEs to fast and slow subsystems is suggested. The suggested approach is based on the comparative analysis of the magnitudes of the eigenvalues of the matrix $J J^*$, where $J$ is the local Jacobi matrix of the system under consideration. The eigenvectors of this matrix are used for construction of the transformation matrix $Q$. The hierarchy of the decomposition is allowed to vary with time as in the original method described in [56]. As in the original approach [56], 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 equations for slow variables was presented in a simplified form, assuming linear variations of these variables during the time evolution of the fast variables. The results showed advantages of the new approach when compared with the one discussed in [56], both from the point of view of accuracy and CPU efficiency.

6. Conclusions
Modelling of sprays involves modelling of a number of processes which can take place simultaneously at scales which differ by more than 7 orders of magnitude. A summary of the results of the modelling of several such processes is presented, with particular emphasis on sprays in diesel engines used in passenger cars. These include spray penetration, droplet heating and droplet evaporation. The modelling of spray penetration (scales of the order of $3 \times 10^{-2}$ m) is based on equations of mass and momentum conservation of the mixture of droplets and entrained air. It is shown that the well known correlation that the penetration length is proportional to the root square of time, can be generalised to include the corrections to this relationship. At the initial stage of spray penetration the analysis of the process can be based on calculating the trajectories of individual droplets, taking entrainment into account.

The modelling of droplet heating involves scales comparable with a typical droplet diameter $10^{-5}$ m. In the general case, this modelling involves the solution of the heat conduction equation inside droplets and in surrounding gas. Remembering that for typical diesel engine parameters the gas diffusivity is much greater than liquid diffusivity, this solution can be simplified and
based on the assumption that the liquid surface temperature is constant during the time step used in computational fluid dynamics (CFD) codes. The modelling of droplet evaporation, even in a high pressure background gas, requires the solution of the Boltzmann kinetic equation inside the Knudsen layer (thickness about $10^{-7}$ m) with appropriate boundary conditions at the droplet surface and the outer boundary of the Knudsen layer. Recent numerical and asymptotic studies of this problem are reviewed. These studies involve scales comparable with the diameters of individual molecules (about $10^{-9}$ m).

It is confirmed that the dynamic decomposition techniques for solving the stiff system of ordinary differential equations, reported earlier, can be an effective tool in spray modelling applications for CFD codes. Further developments of this technique, based on the comparative analysis of the magnitudes of the eigenvalues of the matrix $JJ^*$, where $J$ is the local Jacobi matrix of the system under consideration, are discussed.

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