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To cite this article: S S Sazhin *et al* 2018 *J. Phys.: Conf. Ser.* **1096** 012052

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# Modelling of sprays: recent results and future challenges

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**Abstract.** A brief overview of some recent developments and future challenges in spray modelling is presented. The focus is on the comparative analysis of Lagrangian and Fully Lagrangian (Osipov) approaches to spray modelling and the applications of the latter approach and its generalisations to the solution of engineering problems, recent developments in modelling the heating and evaporation of spherical and non-spherical droplets and films, and application of the method of integral manifolds in the analysis of spray heating, evaporation and ignition in Internal Combustion (IC) engine-like conditions. Future challenges described in the paper include the generalisation of the Fully Lagrangian approach to enable it to model realistic turbulent sprays, further development of the models of heating and evaporation of deformed droplets, modelling of heating and evaporation of droplets in trans- and super-critical conditions and further development of the integral manifold methods to enable their application to the solution of realistic engineering problems, with particular focus on IC engines. All models are expected to be developed in formats that enable their relatively simple implementation into commercial Computational Fluid Dynamics (CFD) codes.

## 1. Introduction

The modelling of sprays has been extensively studied for over 100 years, and the results have been summarised in numerous publications including [1]. These studies have been stimulated by engineering, environmental and pharmaceutical applications and much progress has been made. The aim of this paper is to summarise the results of those studies that are closest to the research interests of the authors, and identify future challenges. The focus will be on recent progress in the developments of the Fully Lagrangian (Osipov) approach and its application to modelling the dynamics of droplet clouds, modelling the heating and evaporation of spherical and spheroidal droplets and films, and development of new mathematical tools (methods of integral manifolds) for modelling spray heating, evaporation and ignition in individual computational cells. This paper is essentially complementary to monographs [2, 3] and the most recent reviews [4, 5].

In Section 2 the conventional Lagrangian and less well known Fully Lagrangian (Osipov) approaches to modelling sprays are briefly described and some results of recent applications of the latter approach to the solution of engineering problems are summarised. Recent developments to modelling spherical and non-spherical droplets and films are summarised in Section 3. Section 4 considers novel developments in the methods of integral manifolds and their application to

modelling spray heating, evaporation and ignition. Some future challenges in spray modelling are discussed in Section 5.

## 2. Lagrangian versus Fully Lagrangian

The problem of modelling dispersed multiphase flows has been widely discussed in the literature (e.g. [6]) and we do not intend to revisit it here. Our focus will be on relatively rarefied sprays when the mass fraction of liquid droplets is much lower than of the carrier phase. In this case, in most engineering applications, the analysis of spray dynamics is based on the Eulerian-Lagrangian approach in which the Eulerian approach is used for the analysis of the carrier phase (gas) dynamics while the Lagrangian approach is used for the analysis of liquid droplets. This approach is used in all commercial CFD codes known to us, including VECTIS [7] and ANSYS Fluent [8, 9]. In this approach, the trajectories of individual droplets or groups of identical droplets (parcels) are calculated directly in specific cells. Although this approach gives reasonably accurate distributions of droplets in the domain, it is not able to lead to accurate prediction of the distribution of droplet number densities unless trajectories of unrealistically large numbers of droplets are considered.

The latter problem was solved in the method suggested by Osipov [10], which is widely known as the Fully Lagrangian (Osipov) Approach (FLA) [11]. In what follows, the main ideas of this approach, developed for Cartesian coordinates in [12, 13, 14], are briefly summarised.

The FLA, in contrast to the conventional Lagrangian method, describes the time and space evolution of particle/droplet (hereafter referred to as droplet) number densities. The expression for the normalised number density  $n_d$  of droplets along the particle trajectory, can be written as:

$$n_d = \frac{n_0}{|J|}, \quad (1)$$

where  $n_0$  is the initial droplet number density,  $|J|$  is the absolute value of the Jacobian of the Eulerian-Lagrangian transformation. Both  $n_d$  and  $J$  are functions of  $t$  and Lagrangian coordinates  $\{\mathbf{x}_0, t_0\}$  (the starting point of the trajectory),

$$J_{ij} = \left( \frac{\partial x_i}{\partial x_{j0}} \right), \quad (2)$$

where  $x_i$  and  $x_{j0}$  are components of  $\mathbf{x}$  and  $\mathbf{x}_0$ , respectively. For the Stokesian flow approximation we have:

$$\frac{\partial \omega_{ij}}{\partial t} = \beta \left( \frac{\partial u_i}{\partial x_{j0}} - \omega_{ij} \right), \quad (3)$$

$$\omega_{ij} = \frac{\partial J_{ij}}{\partial t} = \frac{\partial v_i}{\partial x_{j0}}. \quad (4)$$

Coefficient  $\beta$  is introduced in the equation

$$\frac{d\mathbf{v}}{dt} = \beta(\mathbf{u} - \mathbf{v}), \quad (5)$$

$\mathbf{x}$  and  $\mathbf{v}$  are the droplet position vector and velocity in Eulerian coordinates,  $u$  is the carrier phase velocity,  $\beta = \tau_d^{-1}$  is the drag force coefficient,  $\tau_d = \frac{\rho_d d_d^2}{18\mu}$ . Equations (4) and (3) can be rewritten as:

$$\frac{\partial J_{ij}}{\partial t} = \omega_{ij} \quad (6)$$

$$\frac{\partial \omega_{ij}}{\partial t} = \beta \left( \sum_k \left( J_{kj} \frac{\partial u_i}{\partial x_k} \right) - \omega_{ij} \right). \quad (7)$$

In the two-dimensional case ( $i, j, k = 1, 2$ ), Equations (6) and (7) are the system of 8 ordinary differential equations with respect to time along the droplet trajectories. At the start of the trajectory, the Lagrangian and Eulerian coordinates are equal. Hence,  $(J_{11})_0 = (J_{22})_0 = 1$ ,  $(J_{12})_0 = (J_{21})_0 = 0$ . Initial values of  $\omega_{ij}$  are inferred from the velocity field of the carrier phase at the starting point assuming that  $x_{j0} = x_j$  in Equation (4). The generalisation of these equations to non-Stokesian flows and cylindrical geometry is straightforward (cf. [10]).

In several of our recent papers the FLA was applied to the analysis of various flows of droplets. In [15], a transient axially symmetric two-phase vortex-ring flow was investigated. The carrier phase parameters were calculated using the approximate analytical solution for the vortex ring suggested in [17]. The vortical nature of the flow in this case is expected to lead to crossings of droplet trajectories which makes the application of the FLA particularly attractive. This approach was used to calculate droplet number densities. Two flow regimes corresponding to two initial conditions were investigated: injection of a two-phase jet and propagation of a vortex ring through a cloud of droplets/particles. The formation of folds and caustics was demonstrated for these flows. The ranges of governing parameters leading to the formation of mushroom-like clouds of droplets were identified. It was shown that the caps of the mushrooms contained caustics or edges of folds of the dispersed media corresponding to droplet accumulation zones.

The results of implementation of the FLA into CFD code ANSYS Fluent and the application of the customised version of this code to the calculation of the number density of inertial droplets in multiphase flows are presented in [16]. Two cases were considered: gas-droplet flow around a cylinder and gas-droplet flow (spray) in a gasoline engine. It was shown that for transient flows with  $Re = 200$  and Stokes numbers greater than about 0.1 around a cylinder the maximal values of droplet number densities predicted by FLA are several orders of magnitude higher than those predicted by a simple model based on the Eulerian/Eulerian approach. This supports application of the FLA rather than a simplified approach for this particular problem.

An application of the FLA to the analysis of a direct injection gasoline fuel spray focused on calculation of the number densities of droplets. Good qualitative agreement between the numerical and experimental results was demonstrated. It was clearly shown that relatively small droplets with diameters  $2 \mu\text{m}$  tend to accumulate in the regions of trajectory intersections, when compared with larger droplets with diameters 10 and  $20 \mu\text{m}$ . This led to the prediction of regions of high number density for small droplets.

The effects of turbulent mixing and droplet inertia on the droplet number density distribution in a turbulent flow field were studied in [18]. In this paper, the turbulent convective diffusion equation for the droplet number density is formulated, based on the modified FLA. It was assumed that droplets with moderate inertia were transported and dispersed by large scale structures of a filtered field in the Large Eddy Simulation framework. It was shown that although turbulent fluctuations are not visible in the filtered solution for the droplet velocity field, they lead to an additional diffusion mass flux and additional dispersion of the droplets. The Lagrangian formulation of the transport equation for the droplet number density and the modified FLA allowed us to resolve the flow regions with intersecting droplet trajectories in the filtered flow field. Thus, the problems of multivalued filtered droplet velocity regions and caustic formation were successfully addressed. The spatial derivatives for the droplet number density were calculated by projecting the FLA solution on the Eulerian mesh. This leads to a hybrid Lagrangian-Eulerian approach to the problem. The main assumptions used in the analysis were supported by calculations of droplet mixing in a transient one-dimensional flow field which was formed by large-scale oscillations with an imposed small-scale modulation. The results of the calculations for droplet mixing in decaying homogeneous and isotropic turbulence were validated by the results of Direct Numerical Simulations (DNS).

### 3. Spherical and non-spherical droplets and films

A detailed review of recent models for mono- and multi-component spherical droplet heating and evaporation is presented in [4]. The models discussed in this review were applied mainly to the analysis of fuel droplets in internal combustion engines. The authors of [19], however, developed a new model for droplet drying based on the previously developed model for multi-component droplet heating and evaporation. This model is based on the previously obtained analytical solutions to the heat transfer and species diffusion equations inside droplets. Small solid particles dispersed in an ambient evaporating liquid, or a non-evaporating substance dissolved in the liquid, were treated as non-evaporating components. Three sub-processes were taken into account in the model for droplet drying: droplet heating/cooling, diffusion of the components inside the droplets, and evaporation of the volatile component. The model was used to analyse the drying of a spray of chitosan dissolved in water. The size of the residual solid ball, predicted by the model after the completion of the drying process, was shown to be consistent with those observed experimentally.

Although considerable progress has been made in the development of models of spherical droplet heating and evaporation, as described in [4, 19], practical application of these models has been limited. The main reason for this is that most droplets observed in engineering applications are far from spherical [20]. The influence of mono-component droplet non-sphericity on their heating and evaporation, approximating droplet shapes as prolate and oblate spheroids, was investigated in [21]. The analytical solutions to heat and mass transfer equations for the gas phase surrounding a spheroidal droplet, previously obtained in [22], were used as boundary conditions for the solutions to these equations in the liquid phase. The temperature gradients inside and at the surface of the droplets, and the changes in their shape during the heating and evaporation process were taken into account. The analysis was based on the assumption that the gradients of temperature and vapour mass fraction along the surface of the droplet are much smaller than those in the direction perpendicular to this surface (slightly deformed droplet). The results were applied to the analysis of heating and evaporation of an n-dodecane fuel droplet in Diesel engine-like conditions. The effect of droplet non-sphericity in these conditions was shown to be relatively small.

A new mathematical model for heating and evaporation of a multi-component liquid film was developed and investigated in [23]. In what follows, the main findings of this paper are briefly summarised.

The model was based on the analytical solutions to the transient one-dimensional heat transfer and species diffusion equations in the liquid phase, subject to the following boundary conditions:

*Liquid/wall interface:*

Wall temperature ( $T_w$ ) is fixed and no species penetrate through the wall:

$$\left. \frac{\partial Y_{1,i}}{\partial x} \right|_{x=0} = 0, \quad (8)$$

where  $Y_{1,i}$  is the mass fraction of the  $i$ th species in the liquid phase,  $x = 0$  refers to the wall/liquid interface.

*Liquid/gas interface:*

The Robin boundary conditions were used for temperature and liquid mass fraction:

$$h(T_{\text{eff}} - T_s) = k_l \left. \frac{\partial T}{\partial x} \right|_{x=\delta_0-0}, \quad (9)$$

$$D_1 \left. \frac{\partial Y_{1,i}}{\partial x} \right|_{x=\delta_0-0} = |\dot{\delta}_{0e}| \left( Y_{1,i}|_{x=\delta_0} - \epsilon_i \right), \quad (10)$$

where

$$T_{\text{eff}} = T_g + \frac{\rho_l L \dot{\delta}_{0e}}{h}, \quad (11)$$

the value of  $\dot{\delta}_{0e}$  (the derivative of the film thickness with respect to time), is controlled by film evaporation,  $|\dot{\delta}_{0e}| = |\dot{m}_e/\rho_l| = h_m \sum_{i=1}^{i=N} \rho_{vsi}/\rho_l$  is the evaporation flux from the surface of the film,  $\rho_{vsi}$  are densities of the  $i$ th vapour species at the outer surface of the film,  $\rho_l$  is the density of the mixture of liquid species,  $L$  is the specific heat of evaporation of the mixture,  $N$  is the total number of evaporating species,

$$\epsilon_i = \frac{Y_{vs,i}}{\sum_{i=1}^{i=N} Y_{vs,i}} = \frac{\rho_{vs,i}}{\sum_{i=1}^{i=N} \rho_{vs,i}}, \quad (12)$$

$Y_{vs,i}$  and  $\rho_{vs,i}$  are the mass fraction and vapour density of the  $i$ th vapour species at the outer surface of the film, respectively. Heat  $h$  and mass  $h_m$  convection heat transfer coefficients were linked by the Chilton-Colburn analogy; the value of  $h$  was assumed constant.

These boundary conditions, supplemented by the standard initial conditions, allowed the authors of [23] to obtain the following analytical solutions to the heat transfer and species diffusion equations.

$$T(X, t) = T_w + \frac{X h_0}{1 + h_0} (T_{\text{eff}} - T_w) + \sum_{n=1}^{\infty} \exp[-\kappa_{\delta 0} \lambda_n^2 t] [q_n + f_n h_0 (T_{\text{eff}} - T_w)] \sin(\lambda_n X), \quad (13)$$

where  $X = x/\delta_0$ ,  $h_0 = h\delta_0/k_l$ ,  $\kappa_{\delta 0} = k_l/(c_l \rho_l \delta_0^2)$ ,

$$q_n = \frac{1}{\|v_n\|^2} \int_0^1 (T_0(X) - T_w) \sin(\lambda_n X) dX, \quad f_n = \frac{1}{\|v_n\|^2} \int_0^1 f(X) \sin(\lambda_n X) dX = -\frac{\sin \lambda_n}{\|v_n\|^2 \lambda_n^2},$$

$f(X) = -X/(1 + h_0)$ ,  $\|v_n\|^2 = \frac{1}{2} \left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{1}{2} \left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right)$ ,  $c_l$ ,  $\rho_l$  and  $k_l$  are specific heat capacity, density and thermal conductivity of the liquid phase, respectively,  $\lambda_n$  are non-trivial solutions to the equation

$$\lambda \cos \lambda + h_0 \sin \lambda = 0. \quad (14)$$

$$Y_{l,i}(t, x) = q_{Y0} \exp \left[ D_1 \left( \frac{\lambda_0}{\delta_0} \right)^2 t \right] \cosh \left( \lambda_0 \frac{x}{\delta_0} \right) + \sum_{n=1}^{\infty} q_{Yn} \exp \left[ -D_1 \left( \frac{\lambda_n}{\delta_0} \right)^2 t \right] \cos \left( \lambda_n \frac{x}{\delta_0} \right) + \epsilon_i, \quad (15)$$

where

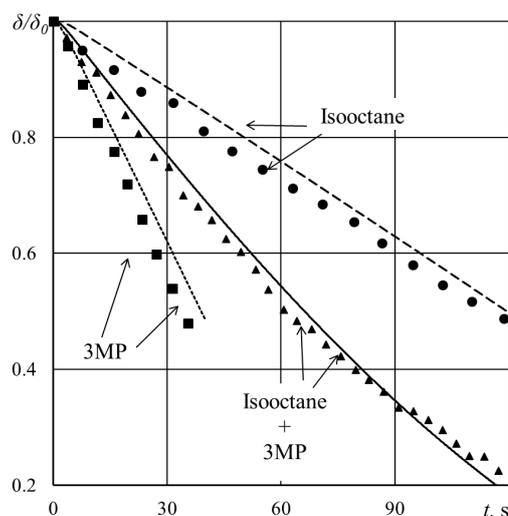
$$q_{Yn} = \frac{1}{\|v_n\|^2} \int_0^{\delta_0} (Y_{l0,i}(x) - \epsilon_i) v_n(x) dx.$$

$D_l$  is the diffusion coefficient of liquid species (assumed to be the same for all species),

$$v_n(x) = \begin{cases} \cosh \left( \lambda_0 \frac{x}{\delta_0} \right) & n = 0 \\ \cos \left( \lambda_n \frac{x}{\delta_0} \right) & n \geq 1, \end{cases} \quad (16)$$

$\lambda_n$  ( $n \geq 0$ ) are the solutions to the following equations:

$$\coth \lambda_0 = \frac{\lambda_0 D_1}{|\dot{\delta}_{0e}| \delta_0}, \quad \cot \lambda_n = -\frac{\lambda_n D_1}{|\dot{\delta}_{0e}| \delta_0} \quad (n \geq 1). \quad (17)$$



**Figure 1.** Time evolution of the film thickness. Circles, triangles and squares show the values obtained in [24]; solid and dashed curves show the predictions of the model. Pure isooctane, pure 3MP, and a 50%/50% mixture of isooctane and 3MP were considered. Reprinted from International Journal of Heat and Mass Transfer, Volume 117, Sazhin et al., A mathematical model for heating and evaporation of a multi-component liquid film, Pages 252-260, Copyright Elsevier (2018).

These equations were supplemented by the standard equations for the gas phase, including the equation for evaporation flux at the film surface and Raoult's law. They were applied at each time step, assuming that the thickness of the film would be constant and the time derivative of this thickness could be inferred from the evaporation rate and thermal swelling. At the end of the time step the thickness was modified to take into account evaporation and swelling. The distribution of temperatures and species mass fractions at the end of the time step were used as the initial conditions for the following time step.

The experimental data presented in [24] were used for validation of the model. In that paper the evaporation of a film composed of mixtures of isooctane/3-methylpentane (3MP) was studied. The results of the comparison for pure isooctane, pure 3MP, and a 50%/50% mixture of isooctane and 3MP are shown in Figure 1. The same input parameters as in [24] ( $T_g = T_w = 302.25$  K,  $T_0(x) = 293.15$  K,  $\delta_0 = 602.72$   $\mu\text{m}$ ) and  $h = 14$  W/(m<sup>2</sup> K) were used in the calculations. As can be seen from Figure 1, the results predicted by the new model are reasonably close to the experimental data for all three cases. This gives us confidence to apply the model to the analysis of other films including those observed in conditions relevant to internal combustion engine systems.

#### 4. Slow invariant manifolds and their application to sprays

The focus of the previous sections was on new methods of analysis of spray dynamics in enclosures (FLA) and the new models of heating and evaporation of droplets and films. Most of these models have already been implemented into the Computational Fluid Dynamics code ANSYS Fluent, and the customised versions of this code have been used for the analysis of specific engineering problems mainly related to automotive applications. The main limitation of these codes is that, although they take into account some of the processes taking place in sprays

(e.g. dynamics of droplets and their heating and evaporation), they overlook a number of other important processes (e.g. chemical reactions in individual cells).

The number of droplets and chemical reactions to be analysed in each cell can be many hundreds and even thousands in the general case, while the number of cells used for the solution of specific engineering problems (e.g. the processes in internal combustion engines) can reach millions (e.g. [7]). These features make it impossible to perform rigorous quantitative analysis of realistic sprays. Two approaches have been developed to deal with this. The first is based on the application of rather simplistic physical models of individual processes, but the geometry of the enclosure is approximated accurately. This approach is used in most CFD codes. The second approach is focused on using accurate physical models of individual processes, ignoring the complexities of the geometry and details of interactions between various processes [2]. These approaches are not contradictory but complementary. In a series of papers (see [2]) a third approach to this modelling was developed. This approach is based on establishing a hierarchy of processes (recognising multiple scales in time and space) and finding a compromise between accuracy and computer efficiency. The models described in the previous sections were developed in line with this.

Another approach to modelling multi-scale spray processes in individual cells could be to use the theory of invariant manifolds, in which the original system of ordinary differential equations for these cells is replaced by other systems on invariant manifolds of lower dimensions. Despite its obvious attractiveness, this method is still rarely used in engineering applications (e.g. [25]). This is mainly attributed to the fact that this approach is based on a number of assumptions, the applicability of which to engineering systems is far from obvious. Also, the mathematical complexity of the theory, and the engineering community's non-familiarity with it, limit its practical application. In what follows, basic ideas of this theory and the most important results of its recent development and application are briefly summarised.

Our focus is on the following autonomous system:

$$\left. \begin{aligned} \dot{x} &= f(x, y) \\ \varepsilon \dot{y} &= g(x, y) \end{aligned} \right\}, \quad (18)$$

where  $0 < \varepsilon \ll 1$ ,  $x \in \mathcal{R}^m$  ( $m$ -dimensional space),  $y \in \mathcal{R}^n$  ( $n$ -dimensional space),  $\mathcal{R}^{m+n} = \mathcal{R}^m \times \mathcal{R}^n$ . Surface  $y = h(x, \varepsilon)$  is called a slow invariant manifold of (18) if any trajectory  $x = x(t, \varepsilon)$ ,  $y = y(t, \varepsilon)$  of (18) having at least one common point  $x = x_0$ ,  $y = y_0$  with the surface  $y = h(x, \varepsilon)$ , i.e.  $y_0 = h(x_0, \varepsilon)$ , lies entirely on this surface, i.e.  $y(t, \varepsilon) = h(x(t, \varepsilon), \varepsilon)$ . This definition is based on the explicit representation  $y = h(x, \varepsilon)$  of the manifold.

A surface  $y = h(x, 0)$  is called a slow manifold (surface). The equation for this manifold can be obtained from the solution to the second equation in System (18) in the limit  $\varepsilon \rightarrow 0$ :

$$g(x, y) = 0. \quad (19)$$

#### 4.1. Smooth case

The formal substitution of function  $h(x, \varepsilon)$  instead of  $y$  into the autonomous system (18) gives the first order partial differential equation (PDE), the so called *invariance equation*,

$$\varepsilon \frac{\partial h}{\partial x} f(x, h(x, \varepsilon), \varepsilon) = g(x, h, \varepsilon) \quad (20)$$

for  $h(x(t), \varepsilon)$ , since  $\varepsilon \dot{y} = \varepsilon \frac{\partial h}{\partial x} \dot{x}$ .

Calculation of function  $h(x, \varepsilon)$  is the key problem when the method of integral manifolds is used to solve specific problems. It is not possible to find explicit forms of this function in the

general case, and various approximations are required. One of these approximations is based on the asymptotic expansion of  $h(x, \varepsilon)$  in powers of small parameter  $\varepsilon$ :

$$h(x, \varepsilon) = \phi(x) + \varepsilon h_1(x) + \dots + \varepsilon^k h_k(x) + \dots \quad (21)$$

Coefficients  $h_1(x), \dots, h_k(x)$  can be found from the invariance equation (20), where  $h(x, 0) = \phi(x)$ , i.e. slow surface  $\phi(x)$  can be considered as a zero-order approximation of the slow invariant manifold. The authors of [30] were the first to use asymptotic expansions of slow invariant manifolds in the form (21).

*4.1.1. Implicit form* If we are not able to find function  $y = \phi(x) = h(x, 0)$  from Equation (19) (which is typical for most engineering applications) then we need to present the equation for it in an implicit form  $g(x, y, 0) = 0$ . In this case the slow invariant manifold can also be obtained in an implicit form (taking into account that  $\varepsilon$  is not zero):

$$G(x, y, \varepsilon) = 0, \quad (22)$$

and the flow on this manifold is described by the first equation in System (18), in which  $x$  and  $y$  satisfy (22). Using the first order approximation, in this case function  $G$  can be found from equation [3]:

$$G_y(x, y, \varepsilon)g(x, y) + \varepsilon G_x(x, y, \varepsilon)f(x, y) = 0. \quad (23)$$

*4.1.2. Parametric form* In many problems, an explicit solution to equation  $g(x, y, 0) = 0$  (zeroth order approximation) can be found in a parametric form:

$$x = \chi_0(v), \quad y = \varphi_0(v),$$

where  $v \in \mathcal{R}^m$ . In this case  $g(\chi_0(v), \varphi_0(v), 0) \equiv 0$  and the slow invariant manifold may also be found in a parametric form:

$$x = \chi(v, \varepsilon), \quad y = \varphi(v, \varepsilon),$$

where  $\chi(v, 0) = \chi_0(v)$ ,  $\varphi(v, 0) = \varphi_0(v)$ .

#### *4.2. Non-Lipschitzian case*

In most cases of the analysis of slow manifolds, including the cases considered in the previous section, it is assumed that all functions are sufficiently smooth and therefore satisfy the Lipschitzian condition [26]:

$$\|g(x_1, y_1) - g(x_2, y_2)\| \leq \mathcal{L}(\|x_1 - x_2\| + \|y_1 - y_2\|), \quad (24)$$

where  $(x_1, y_1), (x_2, y_2)$  are arbitrary arguments from the domain and  $\mathcal{L} > 0$ .

The authors of [28, 29] drew attention to the fact that the order reduction of systems with non-Lipschitzian non-linearities can be performed, using the concept of positively invariant manifolds. In this case, the analysis is focused on the following system:

$$\dot{x} = f(x, y), \quad \dot{y} = \psi(y)g(x, y), \quad (25)$$

where  $x$  and  $y$  are a vector and scalar, respectively; scalar function  $\psi(y)$  is non-Lipschitzian. It is assumed that  $0 < \varphi_1 \leq g(x, y) \leq \varphi_2$  for sufficiently small non-negative values of  $y$ ,  $f(x, y)$  and  $g(x, y)$  are continuous functions.

Let us assume that  $\psi = -y^\alpha$  ( $0 < \alpha < 1$ ). Since the right hand side of this equation for  $y$  in (25) is zero at  $y = 0$ , any trajectory, described by (25), with initial point  $(x_0, 0)$  on the

surface  $y = 0$  lies on this surface for all  $t \geq 0$ . This surface, however, is not invariant since not all trajectories of System (25) which have at least one point in common with the surface lie entirely on it, as trajectories can leave this manifold when  $t$  decreases. This surface, however, is positively invariant and any solution to System (25) with initial point  $(x_0, y_0)$  with sufficiently small positive  $y_0$  reaches the surface during a finite time interval. Moreover, it is attractive. To prove this, the approach suggested in [27] can be used, which considers the Lyapunov function  $V(y) = y^2/2$  with the derivative

$$\dot{V}(y) = -y^{1+\alpha}g(x, y).$$

This derivative is negative for  $y > 0$  for all values of  $x$  under consideration. This implies the asymptotic stability of  $y = 0$  with respect to variable  $y$ , i.e.  $y \rightarrow 0$  as  $t$  increases.

The same analysis can be applied to the case when  $\psi = (\bar{y} - y)^\alpha$ , where  $\bar{y}$  is a positive constant since the change of variable  $z = \bar{y} - y$  leads to the equation  $\dot{z} = -z^\alpha g(x, \bar{y} - z)$ .

This concept was applied to the analysis of spray ignition based on five ODEs (for gas temperature, fuel vapour and oxygen concentrations, and droplet temperatures and radii). This system was reduced to single ordinary differential equations for gas temperature or fuel concentrations. It was shown that the equation for gas temperature predicts an increase in gas temperature up to its limiting value at finite time. Once this happened, then either fuel vapour or oxygen, depending on their initial concentrations, were completely depleted [28].

## 5. Future challenges

### 5.1. Turbulent sprays

The original version of the Fully Lagrangian Approach was developed for the case when the velocity field of the carrier phase is stationary or almost stationary. To the best of our knowledge, the authors of [18] were the first to attempt to generalise this approach to the turbulent carrier phase. The analysis presented in [18] is essentially based on the assumption that the contributions of the droplet velocity fluctuations to the mass and momentum fluxes are both small, but the ratio  $|\mathbf{j}_T|/n_d|\bar{\mathbf{v}}_d|$  is much greater than the ratio  $\overline{v'_{d,i}v'_{d,j}}/\bar{v}_{d,i}^2$ , where  $\mathbf{j}_T$  is the turbulent mass flux of droplets driven by turbulent fluctuations of the carrier phase. The validity of this assumption was proven for a simple one-dimensional flow and droplets with moderate inertia. In the general case, however, the validity of this assumption is far from obvious. This problem needs to be overcome in order to develop a generalised version of the FLA applicable to a wide range of turbulent carrier phase flows.

### 5.2. Deformed droplets

Although some progress in developing models for heating and evaporation of non-spherical droplets have been made [21], the model developed in the latter paper is applicable only to 'slightly' non-spherical droplets (spheroids with eccentricity close to 1). A recent paper by Cossali and Tonini [31] described a new approach to modelling the effect of variable density and diffusion coefficient on heat and mass transfer from a single component spherical droplet evaporating in a high temperature air stream. This approach could potentially lead to the development of a model for strongly deformed spheroidal droplet heating and evaporation. Regardless of the results of this potential development, however, at least two main challenges still remain. Firstly, the droplets are likely to be far from spheroidal [20]. Traditionally the evolution of arbitrary droplet shapes has been modelled using Level Set of Volume of Fluid (VOF) methods (e.g. [32]), but the application of these methods in CFD codes would at present appear to be unrealistic. Secondly, even in the case of slightly deformed spheroidal droplets the model developed in [21] is not ideal for implementation in CFD codes. The creation of a simplified model of the processes, similar to the ones developed for spherical droplets [2], is still a challenge.

### 5.3. Supercritical sprays

The models for spherical and non-spherical droplet heating and evaporation described earlier in the paper are essentially based on the assumption that a sharp interface between liquid and gas can be traced. This is valid only in the case when heating and evaporation of droplets take place in sub-critical conditions. The generalisation of these models to the case of trans- and super-critical conditions, when the interface between the liquid and gas phase becomes blurred [33], is still a challenge.

### 5.4. Integral manifolds in engineering modelling

Although integral manifolds, and their recent use in engineering, have been widely discussed in the literature [29], it is too early to claim that they are a commonly recognised tool of engineering modelling. The main reason for this is that the workhorse of engineering modelling is considered to be the commercial CFD codes, in which these methods are not generally used. A preliminary attempt to combine the methods of integral manifolds with these codes was made in [25], but there have been no further developments in this direction. We believe that this is one of our future challenges.

## 6. References

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### Acknowledgments

S. Sazhin was supported by the EPSRC, UK (grant EP/M002608/1), and the Royal Society (UK) (grant IE 160014). E. Shchepakina was supported by the Ministry of Education and Science of the Russian Federation, as part of the “Research and Development in Priority Areas of Advancement of the Russian Scientific and Technological Complex for 2014-2020” program (Project RFMEFI58716X0033).