

A STUDY OF THE EULERIAN MULTI-FLUID METHOD FOR AN ACCELERATING AND EVAPORATING SPRAY

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ABSTRACT

The Williams spray equation is numerically modelled in this work by the Eulerian multi-fluid method. This equation may be interpreted as a balance equation for the number density of spherical, poly-disperse droplets that are suspended in a gas environment. The physical phenomena of droplet transport, droplet evaporation, droplet heating, acceleration due to drag and gravity forces, collision, coalescence and break-up of droplets are included in this equation and thus it is appropriate for the description of dilute and non-dilute sprays. In this work we focus on the transport, the drag, the evaporation and the heating of dilute sprays. Therefore, the number density depends on time, space, droplet velocity, droplet temperature and an additional variable which is chosen to be the droplet surface. The Eulerian multi-fluid method is based on a finite-volume-like discretisation that conserves the mass and the droplet number in the surface phase-space. The deviation of the numerical model from the exact solution of a simplified spray problem is studied. In addition, the modelling error of the Williams spray equation is assessed by comparing the numerical solution of a refined physical model to an experiment of Wong and Chang [*Int. J. Heat Mass Transfer*, vol. 35, pp. 2403-2411, 1992].

INTRODUCTION

The first objective of this work is to prove the Eulerian multi-fluid method to solve the Williams spray equation [1] with a manageable numerical error. To this end, a form of the spray equation is used that does not take into account collision, coalescence or break-up. This reflects the condition of dilute sprays. The drag force is modelled by the Stokes law and the evaporation rate is kept constant. The one-dimensional version of this problem can be solved analytically and the comparison to the numerical solution gives the exact values of the numerical error the Eulerian multi-fluid method is committing. After having demonstrated the numerical capability of this method, we study the applicability of the Williams spray equation to spray phenomena that include transport of droplets in real space (x,t) , droplet evaporation, droplet heating and acceleration due to drag and gravity forces.

There are several reasons for the need of this study. First of all, the atomization and spray phenomena can be found in a huge number of technical processes and therefore any serious study in this area is of a certain value. There are prominent technical devices that use specific properties of sprays, e.g. in pressure washers the momentum of the spray is used to clean, in spray-coating the spatial homogeneity of the spray allows equal distribution of paint on surfaces or in spray cooling the evaporation of the liquid allows controlling the temperature of hot steel slaps for example. Although this study could also be used to describe and optimise the above devices it is not our first goal. This work can rather be considered as a preliminary work for the prediction of the spray phenomena in technical combustion processes like in IC-engines or gas turbine combustion chambers. For the purpose of limiting the pollutant emission and reducing the fuel consumption in the

combustion of carbon fuels there is an urgent demand to optimise the design of combustion chambers, injection nozzles and cylinders through CFD calculations. So far, the combustion of diesel in IC-engines, for example, can not be captured through CFD calculations because of the challenges to describe (cf. [2])

- i. the atomization process of the liquid fuel in and at the tip of the nozzle,
- ii. the highly transient spray behaviour,
- iii. the highly unsteady motion of the gas mixture away from the nozzle,
- iv. the ignition of the gas mixture,
- v. the complex chemical reaction and
- vi. the coupling of all the above phenomena.

It is therefore reasonable to first tackle the different processes separately and later combine the matured algorithms and methods that result from the detailed studies.

After the fuel is injected and the liquid droplets are formed their behaviour is commonly described by Euler-Lagrangian techniques (cf. Dukowicz [3], R ger et. al. [4], Chrigui et al.[5]). It is based on the tracking of a large number of objects, called parcels, that represent the behaviour of the droplets. For stationary processes good results can be obtained but for unsteady flows this method requires a large number of parcels in order to deliver smooth statistics. In addition, the parallelization technique of dividing the computational domain into several sub domains to compute each of them separately is not very successful because most of the parcels are concentrated near the nozzle. The desired linear scaling of the computational time with the used processors can not be easily achieved.

The use of large-eddy simulations (LES) is essential for the description of the gas turbulence in combustion processes because the dominating effects, i.e. the injection, the flow and the combustion, are highly unsteady. We therefore argue that an Eulerian description of the droplet behaviour coupled to the LES gas-solver is advantageous to capture the unsteady behaviour of the considered motion without increasing the computational effort. In contrast to the parcel tracking of the Euler-Lagrange method the equations for the Eulerian description of the droplets have to be solved for the temperature and the densities of droplet number, mass and momentum at every point in the domain. For an overview of the recent advances in this field see Massot [6] or Kaufmann [7]. In this work we choose an Eulerian approach, coined by Laurent et al. [8] ‘‘Eulerian multi-fluid method’’, that is able to describe poly-disperse sprays that undergo evaporation, collision, coalescence and break-up. This method was originally suggested by Greenberg et al. [9], rigorously defined by Laurent, Massot and Villedieu [10, 8] and extended to second-order in surface phase-space by Dufour and Villedieu [11]. In this work we will use the second-order approach of Dufour and Villedieu.

The remainder of this paper is organized as follows. In the second part we introduce Williams Spray equation, specify the different models for drag, evaporation etc., and strip the emerging equation from its dimension. We also present the main ideas of the Eulerian multi-fluid method. In a third section the numerical aspects of this method are outlined. The fourth section is devoted to the comparison of the numerical method to an analytical solution and the experimental measurements of Wong and Chang [12]. We conclude this article by summarising the achievements of this work and by giving an outlook.

DEFINITIONS AND THEORY

Physical model of a dilute spray

It is not uncommon that technical spray systems consist of millions of fluid droplets of size 10-100 μm suspended in a moving gas environment. Here, the behaviour of droplets and its interaction with the surrounding gas is modelled by the, so-called, Williams spray equation [1] which is closely related to the kinetic gas theory (cf. Boltzmann [13]). It has the general form

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{\partial}{\partial \mathbf{x}}(\mathbf{v}f) + \frac{\partial}{\partial \mathbf{v}}(\mathbf{F}f) + \frac{\partial}{\partial s}(\mathbf{K}f) \\ + \frac{\partial}{\partial \theta}(\mathbf{R}f) = \Gamma(f) + \Theta(f), \end{aligned} \quad (1)$$

where f is a function of time t , space \mathbf{x} , velocity \mathbf{v} , a scalar that characterizes the droplet size s (here, the surface) and the temperature θ . It is physically interpreted as number density of the droplets per infinitesimal volume $([dx_1, dx_2] \times [dv_1, dv_2] \times [ds_1, ds_2] \times [d\theta_1, d\theta_2])$. In Eq.(1), the first two terms on the left hand side represent the free transport of a droplet with velocity \mathbf{v} , followed by a term that includes the forces \mathbf{F} which affect a droplet. The last term in the first row of Eq.(1) accounts for the continuous changes of the droplet size and the last term on the left hand

side reflects the temperature changes of the droplets. Γ and Θ allow for the consideration of discontinuous interactions between the droplets, the breakage of one fluid object into several others or inversely the collision and coalescence of droplets, respectively. \mathbf{F} , \mathbf{K} and \mathbf{R} take into account the interaction with the gaseous phase and are modelled as follows.

For \mathbf{F} , fancy models exist for all kinds of special applications. By taking into account the large ratio of droplet density vs. gas density, arguments of dimensional analysis lead to the expression

$$\mathbf{F} = \frac{\mathbf{U}_g - \mathbf{v}}{\tau_d(s, \mathbf{v})} + \mathbf{g} \mathbf{e}_g \quad (2)$$

where \mathbf{U}_g is the gas velocity, τ_d the relaxation time that contains the information on the shape of the droplet and $\mathbf{g} \mathbf{e}_g$ represents the acceleration vector which is due to gravity. The relaxation time is related to the particle drag coefficient C_d via

$$\frac{1}{\tau_d} = \frac{3\sqrt{\pi}}{4} \frac{\rho_g}{\rho_d} C_d s^{-1/2} \|\mathbf{U}_g - \mathbf{v}\|. \quad (3)$$

We refer to ρ_g as the constant mass density of the gas and to ρ_d as that of the droplets. Different expressions exist for the particle drag coefficient depending on the application and the desired degree of complexity. Stokes assumed the simple form

$$C_d = \frac{24}{\text{Re}_d}, \quad \tau_d(s) = \frac{\rho_d s}{18\pi\mu_g} \quad (4)$$

and Schiller and Naumann [14] extended this form to

$$C_d = \frac{24}{\text{Re}_d} \left(1 + \frac{1}{6} \text{Re}_d^{2/3} \right) \quad (5)$$

for more elevated Reynolds numbers,

$$\text{Re}_d = \frac{s^{1/2} \|\mathbf{U}_g - \mathbf{v}\|}{\nu_d \sqrt{\pi}}. \quad (6)$$

The kinematic viscosity of the droplets, ν_d , and the dynamic viscosity of the gas, μ_g , are assumed to be constant. We regard \mathbf{U}_g as well as the vapour mass fractions, Y_v , the mass fraction of the ‘‘dry’’ gas, Y_a , and the temperature of the gas, θ_g , to be supplied by a multi-component flow solver for the gas motion.

The ‘‘velocity’’ of the evaporation, \mathbf{K} , is defined by

$$\frac{\partial s}{\partial t} = \mathbf{K}, \quad (7)$$

where \mathbf{K} is negative for evaporation. For spherical droplets \mathbf{K} is related to the usual mass transfer $\dot{m}_v = \partial m_d / \partial t$ via

$$\mathbf{K}(\mathbf{v}, s) = \frac{6\sqrt{\pi}}{\rho_d s^{3/2}} \dot{m}_v(\mathbf{v}, s). \quad (8)$$

Following the uniform temperature model of Abramzon and Sirignano [15] we assume the mass transfer to have the form

$$\dot{m}_v(\mathbf{v}, s) = \sqrt{\pi} s^{1/2} \rho_g D_{va} Sh_{0,mod} \ln(1 + B_m). \quad (9)$$

The reader is again referred to Abramzon and Sirignano [15] or to Ochs [16] for the detailed expression for the modified Sherwood number, $Sh_{0,mod}$ and the mass transport number,

$B_m \cdot D_{va}$ represents the diffusivity of the fuel vapour in the surrounding gas.

The change of the droplet temperature is due to two physical effects. First, the temperature difference between droplet and gas that leads to an heat flux, \dot{Q}_s , crossing the droplet surface. Second, the change of phase of the droplet liquid is a process of negative heat balance. The measure for the heat sink is the latent heat Δh_v which depends on the temperature at the droplet surface in the gas phase. Again, we draw on the model of Abramzon and Sirignano [15] to define the heat flux. The final representation of the temperature change, \mathbf{R} , has the form

$$\mathbf{R}(\mathbf{v}, \theta, s) = \frac{\dot{m}_v(\mathbf{v}, s)}{c_{p,d} m_d(s)} \left(\frac{c_{p,v}}{B_h} (\theta_g - \theta) + \Delta h_v \right), \quad (10)$$

where we assumed the droplets to have a uniform temperature. The heat transfer number, B_h , can be computed by an iterative procedure proposed by Abramzon and Sirignano [15]. Again, the values of the specific heat capacities $c_{p,d}$ for the droplet and $c_{p,v}$ for the vapour are material depended. They can be found elsewhere (cf. VDI-Wärmeatlas [17]). The quantity m_d represents the mass of a droplet.

Although the effects of coalescence and breakage of droplets can be described by the Williams spray equation and could also be tackled by the Eulerian multi-fluid method we are not considering these effects in the present study. Therefore, we are not dealing with dense sprays.

Let us now strip the dimensions from Eq.(1). To this end, we define the non-dimensional variables

$$\begin{aligned} t &= \tau_g t^*, \quad \mathbf{x} = \lambda \mathbf{x}^*, \quad \mathbf{v} = A \mathbf{v}^*, \quad \mathbf{U}_g = A \mathbf{U}_g^*, \\ s &= S_{ref} s^*, \quad \theta = \theta_{ref} \theta^*, \end{aligned} \quad (11)$$

with the characteristic length, velocity and time scale for the gas flow λ , A and $\tau_g = \lambda/A$, respectively. S_{ref} represents

a characteristic size of the droplets which is taken to be the surface of the largest droplet. The reference temperature, θ_{ref} , is set equal to a characteristic gas temperature θ_g . The non-dimensional form of f can be deduced from its interpretation mentioned earlier. It reads

$$f^*(t^*, \mathbf{x}^*, \mathbf{v}^*, s^*, \theta^*) = f(t, \mathbf{x}, \mathbf{v}, s, \theta) \lambda^3 A^3 S_{ref} \theta_{ref}. \quad (12)$$

In addition, we define the time scales

$$\tau_{evap} = -\frac{S_{ref}}{\mathbf{K}}, \quad \tau_{heat} = \frac{\theta_{ref}}{\mathbf{R}}, \quad (13)$$

and the non-dimensional numbers for evaporation and heat transfer as well as the Stokes number and the Froude number by

$$E_v = \frac{\tau_g}{\tau_{evap}} \geq 0, \quad H_{eat} = \frac{\tau_g}{\tau_{heat}}, \quad (14)$$

$$St(s^*, \mathbf{v}^*) = \frac{\tau_d}{\tau_g} \quad \text{and} \quad Fr = \frac{A}{\tau_g g},$$

respectively. With these definitions we obtain the non-dimensional Williams spray equation

$$\begin{aligned} &\frac{\partial}{\partial t}(f) + \frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{v}f) \\ &+ \frac{\partial}{\partial \mathbf{v}} \cdot \left\{ \left(\frac{\mathbf{U}_g - \mathbf{v}}{St(\mathbf{v}, s)} + \frac{1}{Fr} \mathbf{e}_g \right) f \right\} \\ &- \frac{\partial}{\partial s}(E_v f) + \frac{\partial}{\partial \theta}(H_{eat} f) = 0, \end{aligned} \quad (15)$$

where symbols $(\cdot)^*$ are dropped hereafter.

Eulerian multi-fluid method

This section is entirely based on the work of Massot and Laurent [10], Laurent et al. [8] and Villedieu and Dufour [11]. As the complete derivations and proofs can be found in these references we will only outline the main ideas of this method.

In the most general case the number density function, f , has, apart from its dependencies on \mathbf{x} and t , $d+2$ degrees of freedom, i.e. the surface and temperature variable and the d velocity components, v_1, \dots, v_d . To reduce the number of free variables we first perform a moment transform of Eq.(15) with respect to all velocity components and the temperature over the whole domain \mathbf{V}^{d+1} . To this end, we define the moments

$$\begin{aligned}
M_{0,0}(t, \mathbf{x}, s) &= \int_{V^{d+1}} f(t, \mathbf{x}, \mathbf{v}, s) d\mathbf{v}d\theta, \\
M_{0,1}(t, \mathbf{x}, s) &= \int_{V^{d+1}} \theta f(t, \mathbf{x}, \mathbf{v}, s) d\mathbf{v}d\theta, \\
\mathbf{M}_{1,0}(t, \mathbf{x}, s) &= \int_{V^{d+1}} \mathbf{v}f(t, \mathbf{x}, \mathbf{v}, s) d\mathbf{v}d\theta.
\end{aligned} \tag{16}$$

The evolution equations for these moments are obtained from Eq.(15) and read

$$\begin{aligned}
\frac{\partial}{\partial t}(M_{0,0}) + \frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{M}_{1,0}) - \frac{\partial}{\partial s} \int_{V^{d+1}} E_v f d\mathbf{v}d\theta &= 0, \\
\frac{\partial}{\partial t}(\mathbf{M}_{1,0}) + \frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{M}_{2,0}) - \frac{\partial}{\partial s} \int_{V^{d+1}} \mathbf{v}E_v f d\mathbf{v}d\theta \\
- M_{0,0} \left(\frac{\mathbf{U}_g - \bar{\mathbf{v}}}{St(\bar{\mathbf{v}}, s)} + \frac{1}{Fr} \mathbf{e}_g \right) &= 0,
\end{aligned} \tag{17}$$

$$\begin{aligned}
\frac{\partial}{\partial t}(M_{0,1}) + \frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{M}_{1,1}) - \frac{\partial}{\partial s} \int_{V^{d+1}} \theta E_v f d\mathbf{v}d\theta \\
- M_{0,0} H_{eat}(\bar{\mathbf{v}}, s, \bar{\theta}) &= 0.
\end{aligned}$$

For the derivation of these equations several assumptions have been used among which the most restrictive one is the following.

There is no dispersion around the mean values of velocity, $\bar{\mathbf{v}}(t, \mathbf{x}, s)$, and temperature, $\bar{\theta}(t, \mathbf{x}, s)$,

i.e. the number density function has the form

$$f = M_{0,0} \delta(\mathbf{v} - \bar{\mathbf{v}}) \delta(\theta - \bar{\theta}). \tag{18}$$

First, we have to remark that with assumption (18) the second velocity moment can be expressed as

$$\mathbf{M}_{2,0} = M_{0,0} \bar{\mathbf{v}} \otimes \bar{\mathbf{v}}, \tag{19}$$

which closes system (17) with regard to the velocity. We also have to point out that assumption (18) still allows a dependency of the velocity on the surface variable s provided we interpret (17)₂ as an equation for the droplet momentum and $\bar{\mathbf{v}}$ as the corresponding velocity. We also observe that for the six free variables in Eq. (17) there are only five equations available.

In this paragraph we use the ideas of Dufour and Villedieu [11] to close Eq. (17) with respect to the variable s . To this end, we subdivide the surface phase-space into N sections $I_i = [s_i, s_{i+1}]$, ($i = 1, \dots, N$) and perform a moment transform with respect to the s in each of these sections. The emerging moments

$$\begin{aligned}
n_i(t, \mathbf{x}) &= \frac{1}{\Delta s_i} \int_{s_i}^{s_{i+1}} M_{0,0}(t, \mathbf{x}, s) ds, \\
m_i(t, \mathbf{x}) &= \frac{1}{\Delta s_i} \int_{s_i}^{s_{i+1}} s^{3/2} M_{0,0}(t, \mathbf{x}, s) ds,
\end{aligned} \tag{20}$$

are interpreted as number and mass density of droplets per section I_i , respectively. In definitions (20) we use the abbreviation $\Delta s_i = (s_{i+1} - s_i)$. The quantity m_i can be interpreted as mass because it is linear to the true, dimensional mass density in one section. The relation reads

$$(m_{true})_i = \frac{\rho_d S_{ref}^{3/2}}{6\sqrt{\pi}} m_i^*(t^*, \mathbf{x}^*), \tag{21}$$

where m_i^* is the quantity defined in Eq.(20). We also define the non-dimensional velocities and temperatures for each section by

$$\begin{aligned}
\mathbf{v}_i(t, \mathbf{x}) &= \frac{1}{m_i} \int_{s_i}^{s_{i+1}} s^{3/2} M_{1,0}(t, \mathbf{x}, s) ds, \\
\theta_i(t, \mathbf{x}) &= \frac{1}{m_i} \int_{s_i}^{s_{i+1}} s^{3/2} M_{0,1}(t, \mathbf{x}, s) ds,
\end{aligned} \tag{22}$$

which are constant in each section I_i . The equations that follow from the moment transform of (17) and definitions (20) and (22) read

$$\begin{aligned}
\frac{\partial}{\partial t}(n_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (n_i \mathbf{v}_i) - \int_{s_i}^{s_{i+1}} \frac{\partial}{\partial s} (E_v M_{0,0}) ds &= 0, \\
\frac{\partial}{\partial t}(m_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (m_i \mathbf{v}_i) - \int_{s_i}^{s_{i+1}} s^{3/2} \frac{\partial}{\partial s} (E_v M_{0,0}) ds &= 0, \\
\frac{\partial}{\partial t}(m_i \mathbf{v}_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (m_i \mathbf{v}_i \otimes \mathbf{v}_i) - \int_{s_i}^{s_{i+1}} s^{3/2} \frac{\partial}{\partial s} (E_v M_{0,0} \bar{\mathbf{v}}) ds \\
- \int_{s_i}^{s_{i+1}} s^{3/2} M_{0,0} \left(\frac{\mathbf{U}_g - \bar{\mathbf{v}}}{St(\bar{\mathbf{v}}, s)} + \frac{1}{Fr} \mathbf{e}_g \right) ds &= 0, \\
\frac{\partial}{\partial t}(m_i \theta_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (m_i \theta_i \mathbf{v}_i) - \int_{s_i}^{s_{i+1}} s^{3/2} \frac{\partial}{\partial s} (E_v M_{0,0} \bar{\theta}) ds \\
- \int_{s_i}^{s_{i+1}} s^{3/2} M_{0,0} H_{eat}(\bar{\mathbf{v}}, s, \bar{\theta}) ds &= 0.
\end{aligned} \tag{23}$$

These equations are considered as the balance equations of number density, mass density, momentum and enthalpy of the droplets in each section. The first two terms in each equation of (23) represent the convection of the respective quantity. Still, this system is unclosed because an expression for $M_{0,0}$

is missing. Dufour and Villedieu [11] proposed an exponential function of the form

$$\tilde{M}_{0,0}(t, \mathbf{x}, s) = \sum_{i=1}^N \mathbf{1}_{s_i < s \leq s_{i+1}} a_i(t, \mathbf{x}) \exp(-b_i(t, \mathbf{x})s) \quad (24)$$

that is defined in such a way that in each section, \tilde{n}_i and \tilde{m}_i obtained from $\tilde{M}_{0,0}$ agree with n_i and m_i originating from the exact $M_{0,0}$. This definition allows us to compute the parameters a_i and b_i by solving the equations

$$n_i = \int_{s_i}^{s_{i+1}} a_i \exp(-b_i s) ds, \quad m_i = \int_{s_i}^{s_{i+1}} s^{3/2} a_i \exp(-b_i s) ds. \quad (25)$$

We first remark that expression (24) allows the evaluation of the integrals arising in Eqs.(23). Second, it was proven (see [11]) that this ansatz leads to a second order description of the evaporation. It also satisfies a maximum principle on the velocities, \mathbf{v}_i , in each section. The finite-volume discretisation of the surface phase-space will be outlined in the next section.

NUMERICAL MODEL

Equations (23) supplemented by (24) are solved using the fractional step method developed by Strang (see LeVeque [18] and references therein). We choose to solve the following systems. First, the equation system for the transport part

$$\begin{aligned} \frac{\partial}{\partial t}(n_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (n_i \mathbf{v}_i) &= 0, \\ \frac{\partial}{\partial t}(m_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (m_i \mathbf{v}_i) &= 0, \\ \frac{\partial}{\partial t}(m_i \mathbf{v}_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (m_i \mathbf{v}_i \otimes \mathbf{v}_i) &= 0, \\ \frac{\partial}{\partial t}(m_i \theta_i) + \frac{\partial}{\partial \mathbf{x}} \cdot (m_i \theta_i \mathbf{v}_i) &= 0, \end{aligned} \quad (26)$$

can be regarded as a weakly hyperbolic system because no pressure term is arising in this system. The second system only considers the influence of the forces on the droplets and the heating. It has the form

$$\begin{aligned} \frac{\partial}{\partial t}(n_i) &= 0, \quad \frac{\partial}{\partial t}(m_i) = 0, \\ \frac{\partial}{\partial t}(m_i \mathbf{v}_i) &= \int_{s_i}^{s_{i+1}} s^{3/2} M_{0,0} \left(\frac{\mathbf{U}_g - \bar{\mathbf{v}}}{St(\bar{\mathbf{v}}, s)} + \frac{1}{Fr} \mathbf{e}_g \right) ds, \quad (27) \\ \frac{\partial}{\partial t}(m_i \theta_i) &= \int_{s_i}^{s_{i+1}} s^{3/2} M_{0,0} H_{eat}(\bar{\mathbf{v}}, s, \bar{\theta}) ds. \end{aligned}$$

The system for the evaporation reads as follows

$$\begin{aligned} \frac{\partial}{\partial t}(n_i) &= \int_{s_i}^{s_{i+1}} \frac{\partial}{\partial s} (E_v M_{0,0}) ds, \\ \frac{\partial}{\partial t}(m_i) &= \int_{s_i}^{s_{i+1}} s^{3/2} \frac{\partial}{\partial s} (E_v M_{0,0}) ds, \\ \frac{\partial}{\partial t}(m_i \mathbf{v}_i) &= \int_{s_i}^{s_{i+1}} s^{3/2} \frac{\partial}{\partial s} (E_v M_{0,0} \bar{\mathbf{v}}) ds, \\ \frac{\partial}{\partial t}(m_i \theta_i) &= \int_{s_i}^{s_{i+1}} s^{3/2} \frac{\partial}{\partial s} (E_v M_{0,0} \bar{\theta}) ds. \end{aligned} \quad (28)$$

We obtain a numerical solution of Eqs.(23) by solving systems (26)-(28) in the following sequence: dt/2 transport – dt/2 drag and heating – dt evaporation – dt/2 drag and heating – dt/2 transport. For each of these steps the solution of the previous step is used as “initial condition” but for the first fractional step the solution of the previous time-step or the initial condition of the problem is taken into account. The solution of the last fractional step is also the solution of system (23) at time $t_n + dt$.

For the numerical treatment of the fractional steps different numerical methods are used. The transport system (26) is discretised by the second order finite-volume scheme of Bouchut [19] which was designed for pressure-less gas equations. For the advancement in time the ODE-solver ODEPACK is incorporated. It was written by Hindmarsh [20] and is also applicable to stiff ODE systems. The same package is used for the solution of the momentum and temperature equation in Eqs. (27). If we chose to model the drag force by the Stokes law, the momentum equation can also be solved analytically.

At first sight, it is not obvious how to derive the desired finite-volume discretisation for equations (28). We therefore return to the Williams spray equation (15) which reduces to the hyperbolic equation

$$\begin{aligned} \frac{\partial}{\partial t}(f(t, s)) - \frac{\partial}{\partial s} (E_v f(t, s)) &= 0, \\ f(t = t_n) &= f^n \end{aligned} \quad (29)$$

for the case of evaporation only. If we assume E_v to be constant during one time step, we easily obtain the solution $f(s, t_n + dt) = f^n(s + E_v dt)$. With this solution and definition (20)₁ the number density at the next time step can be written as

$$n_i(t_{n+1}) = \frac{1}{\Delta s_i} \int_{s_i}^{s_{i+1}} \int_{\mathbf{v}^{d+1}} f^n(s + E_v dt, \mathbf{v}, \theta) d\mathbf{v} d\theta ds, \quad (30)$$

where all quantities on the right hand side are known from the previous fractional step. With some algebra Eq.(30) can be transformed into the standard form

$$n_i(t_{n+1}) = n_i(t_n) + \frac{E_v dt}{\Delta s_i} \left[F(n_i^n, n_{i+1}^n) - F(n_{i-1}^n, n_i^n) \right] \quad (31)$$

of a conservative finite-volume scheme in the surface phase-space. The fluxes F can be derived from Eq.(30). Equivalent expressions can be found for the quantities m_i , $m_i \mathbf{v}_i$ and $m_i \theta_i$ defined in (20) and (22).

RESULTS

Study of the numerical model

In this section we study the numerical error of the Eulerian multi-fluid method by comparing it to an analytical solution of a reduced spray problem. Obviously, model (15) does not allow any analytical treatment, unless we reduce the complexity of the incorporated physical models and limit the number of variables without ignoring all physical effects. We first reduce the number of variables of f by considering the stationary and isothermal case, i.e. t and θ are dropped from the argument list of f . We also assume that the discontinuous interactions between the droplets are not significant and the droplets do evaporate according a law, that allows E_v to be a constant. By reducing the problem to one dimension in space we obtain equation

$$\frac{\partial}{\partial x}(vf) + \frac{\partial}{\partial v} \left(\frac{U_g - v}{St(v, s)} f \right) - E_v \frac{\partial}{\partial s}(f) = 0, \quad (32)$$

where in the case of the Stokes law the Stokes number is linear in s with a factor $\alpha = \rho_d S_{ref} / 18 \pi \mu_g \tau_g$ that represents the Stokes number of the largest droplet. We complete this mathematical problem by defining the boundary condition

$$f(x=0, v, s) = f_0(v, s), \quad (33)$$

with the inflow distribution f_0 . It is assumed that at the inflow (but only there) the droplets have the same velocity and that $s > 0$. The method of characteristics leads to a semi-analytical solution. Certain integrals have to be solved with numerical quadrature schemes. In this work there is no room to show the detailed derivation of the solution (cf. Dufour and Villedieu [11]). We therefore omit the algebraic expression of the solution and only illustrate the non-dimensional Sauter mean diameter, d_{32} , and the total densities of mass, m_{sys} , and number, n_{sys} , of droplets in Fig. 1 and 2, respectively.

In Fig. 1 the analytical solution is plotted versus the numerical solution of the Sauter mean diameter for three different numbers of sections. It is observed that with increasing number of sections the analytical solution is very well represented and only tiny numerical errors are observed for the case of 20 sections. Although, we have used very

restrictive models for evaporation and drag, still we have demonstrated that the Eulerian multi-fluid method can reproduce the analytical solution, a necessary condition to apply it to more complex spray problems. With Fig. 2 we want to demonstrate that even for the solution with seven sections, the numerical error committed for the mass density and the number density is not significant. This observation results from the comparison of Fig. 1 to Fig. 2. We observe that in that area where the solutions are deviating from the analytical solution (Fig. 1), Fig. 2 shows that there is not much mass left that may be represented by a wrong Sauter diameter.

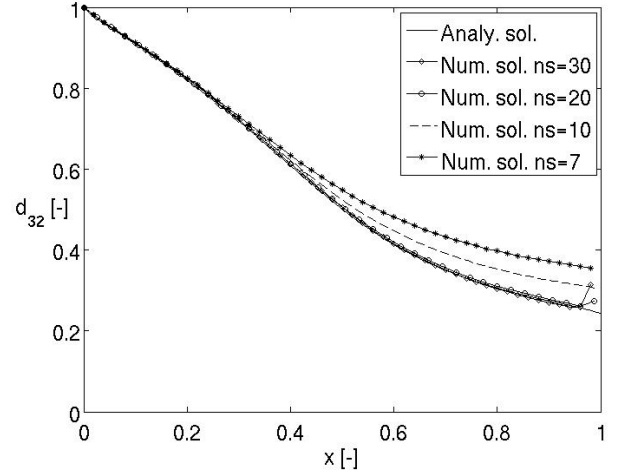


Fig. 1 Sauter mean diameter vs. position for the simplified spray problem

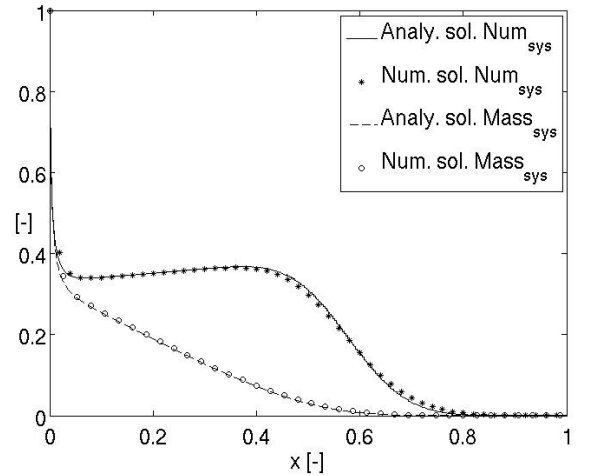


Fig. 2: Total mass and number density vs. position

Study of the physical model

In order to justify the physical models presented in the second section we compare calculations of the Eulerian multi-fluid method to the axis-symmetric evaporation experiment of Wong and Chang [12]. They considered a vaporising Tetralin ($C_{10}H_{10}$) spray that exhibits acceleration, heating and evaporation in a slowly moving N_2 gas stream through a cylindrical tube which is facing in the direction of gravity. At the entrance of the tube the poly-disperse spray has approx. a velocity of 0.9 m/s, a temperature of 35° C and a Sauter mean diameter of 60 μm . Here, it is assumed that the properties of the surrounding gas, i.e. the velocity of 1 m/s, the temperature

of 75° C and the mass fraction of Tetralin vapour are constant along the longitudinal axis. This strong assumption reduces the simulation effort significantly but reduces the value of the results, especially for less dilute sprays where the saturation of the gas is reached in the tube. In Fig. 3 the remaining volume fraction of the droplets at the middle axis is plotted together with the one dimensional solution of the Eulerian multi-fluid method. In the case where all particles are considered to compute the remaining volume fraction there is no region where the deviation of the normalised results from the experiment and the numerical solution is small. There may be several reasons for these deviations. We have already mentioned that it is indispensable to take into account the influence of the droplets on the gas in order to capture at least the saturation of the gas and the reduction of the gas temperature. On the other hand, due to the limitations of the measurement technique, the volume fraction of the small droplets is not captured. In Fig. 3 we also show a plot of the Eulerian multi-fluid method that is omitting the small particles ($d < 20 \mu\text{m}$) on purpose. The much better agreement should not hide the fact that a two-way coupling between spray and gas is necessary to achieve acceptable predictions of this type of flow.

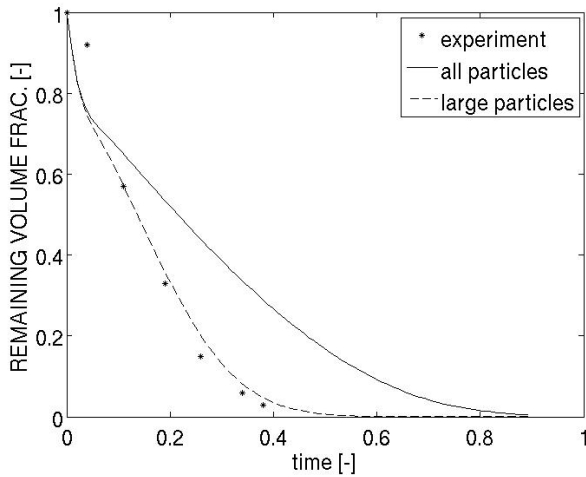


Fig. 3: Remaining volume fraction vs. averaged time, measured [12]; calculated with 20 sections considering all particles and only particles with diameter larger than $20 \mu\text{m}$.

CONCLUSION

In this study it has been demonstrated that the second order Eulerian multi-fluid method can compute the Williams spray equation with a high degree of accuracy. The reduction of the number of sections which may be necessary in order to reduce the computational effort, still allows numerical solutions with acceptable error in the prediction of the remaining fluid mass. From the comparison of a well resolved numerical solution with the experiment of Wong and Chang [12] it is concluded that the influence of the droplets on the gas have to be considered in any case also for dilute sprays. Further increasing the density of the droplets leads to effects like collision and coalescence which, in principle (cf. Laurent et al. [8]), can also be captured by the Eulerian multi-fluid method. The effect of droplet break-up which is more pronounced for large droplet-gas momentum differences and for high Weber numbers is planned to be implemented in the code used here. The capability of this method to predict unsteady spray phenomena is another task that will attract our attention in future works. This work is the first step in a series

of studies that are performed to rigorously implement the Eulerian multi-fluid method.

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NOMENCLATURE

Symbol	Quantity	SI Unit
A	Char. gas velocity	m/s
a_i	Parameter in density function f	-
B_h	Heat transfer number	-
B_m	Mass transfer number	-
b_z	Parameter in density function f	-
C_d	Particle drag coefficient	-
c_{pd}	heat capacity of liquid	kJ/kg K
c_{pv}	heat capacity of vapour	kJ/kg K
dt	Numerical time step	s, - after p.3
D_{va}	Diffusivity	m^2/s
E_v	Non-dimensional number for evaporation	-
\mathbf{e}_g	Direction of gravity	-, unit normal
\mathbf{F}	Drag and gravity force	m/s^2
Fr	Froude number	-
f	Number density function	$\text{s}^3/\text{m}^8 \text{K}$
g	Gravity constant	m/s^2
H_{eat}	Non-dimensional number for heat transfer	-
I_i	Section i	-
K	Evaporation function	m^2/s
$M_{i,j}$	Mixed moment, i-th order velocity, j-th order temperature	-
m_i	Mass density of droplets in section i	-
m_d	Mass of a spherical droplet	kg
\dot{m}_d	Mass transfer	kg/s
N	Number of sections	-
n_i	Number density of droplets in section i	-
\dot{Q}_s	Heat flux between gas and droplets	J/s
R	Heating function	K/s
Re_d	Droplet Reynolds number	-
S_{ref}	Referential surface size	m^2
$Sh_{0,\text{mod}}$	Modified Sherwood number	-
St	Stokes number	-
s	Surface variable	m^2 , - after p.3
t, t_n	Time	s, - after p.3
\mathbf{U}_g, U_g	Gas velocity	m/s, - after p.3
\mathbf{v}, v	Droplet velocity	m/s, - after p.3
$\bar{\mathbf{v}}$	Mean velocity	-
\mathbf{v}_i	Droplet velocity in section i	-
\mathbf{x}, x	Distance	m, - after p.3
Y_v	Vapour mass fraction	-
Y_a	“Dry” gas mass fraction	-
Γ	Breakup function	$\text{s}^2/\text{m}^8 \text{K}$
Δs_i	Size of section I_i	m^2 , - after p.3
Θ	Collision and coalescence function	$\text{s}^2/\text{m}^8 \text{K}$

θ	Temperature variable	K, - after p.3
θ_g	Gas variable	K, - after p.3
θ_{ref}	Referential temperature	K
θ_i	Temperature in section I_i	-
$\bar{\theta}$	Mean temperature	-
λ	Char. length scale for the gas	m
μ_g	Dynamic viscosity of the gas	kg/m s
ν_d	Kinematic viscosity of the droplet	m ² /s
φ_d, φ_g	Density of droplet and gas	kg/m ³
τ_d	Droplet relaxation time	s
τ_g	Charc. time for the gas	s
τ_{evap}	Evaporation time	s
τ_{heat}	Heating time	s

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