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## A new high order moment method for polydisperse evaporating sprays dedicated to the coupling with separated two-phase flows in automotive engine

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### Abstract

Liquid fuel injection modeling and simulation in automotive engines face new challenges related to the need for predictive simulations of combustion regimes. Recently, derived from a statistical approach at mesoscopic level, a high order method of moments coupled to realizable, robust and accurate numerical methods [1], has been obtained and shown to describe properly the dynamics of polydisperse evaporating sprays and its coupling to a turbulent gaseous flow field [2]. However, building up a global multi-scale model with the capability to resolve the whole injection process requires a major breakthrough in terms of both modeling and numerical methods. A new model for evaporating polydisperse sprays with easy coupling capabilities to the separated phases zone is proposed in the present contribution, as well as specific numerical methods and implementation in the `p4est` library [3] for adaptive mesh refinement and massively parallel computing. The key ingredient is a good choice of variables, which can describe both the polydisperse character of a spray as well as the topology of an interface. After verification cases, some two-phase simulations, challenging both in terms of physics and of high performance computing, have been conducted using adaptive mesh refinement [4]. We focus here on a 3D simulation of a spray in the presence of a frozen Homogeneous Isotropic Turbulence (HIT) gaseous carrier flow and assess the ability of the model and of the related numerical methods to capture the physics of such flows.

*Keywords: Two phase flow, polydisperse spray, separated phases, interface topology, moment method*

### 1. Introduction

Direct injection systems are widely used in new automotive engines to improve the air/fuel mixing. Thus, automotive industries have widely improved the engine efficiency, as well as reduced pollutant emissions. In the objective of designing more reliable and efficient injectors, engineers and researchers need predictive numerical modeling in order to understand the complex physics of the flow and also to conduct numerical experiments for the design of new engine prototypes. In particular, the liquid fuel injection and the air-fuel mixture topology play a key role in determining the combustion regime as well as the pollutants formation.

Close after the mouth of the injector, the liquid fuel is injected into the engine at high speed and pressure. At this stage the liquid fuel is separated from the gas by a smooth and thin interface, where the different interactions between the phases take place. In this region, we have to deal with what is called a separated phases two-phase flow. The interaction between the liquid and the surrounding gas increases the interface instabilities and triggers the droplets formation. Finally, this atomization process yields an evaporating polydisperse spray. The challenge is to provide a model as well as a numerical strategy, which are able to describe the whole process and capture the large scale spectrum of such physics and then provide predictive numerical simulations at relatively reasonable computational cost. Deterministic approaches, where a direct numerical simulation of the interface is used for example *tracking methods* (Lagrangian meth-

ods [5], Marker And Cell (MAC) methods [6]) or *interface capturing and reconstruction* (VOF, Level-Set and hybrid method - see [7, 8, 9, 2] and references therein), yield a high computation time and memory requirement, but fail to predict the structure and size distribution of the disperse phase in realistic configurations. Therefore, reduced-order models, where averaging approaches are envisioned, have to be considered since a full resolution is out of reach. Our strategy is to build a reduced-order model for the disperse liquid phase, which is able to resolve the polydisperse character of the spray, by using a set of variables which can be identified as averages of the gas-liquid interface topology.

In this context, we start from a statistical description of the droplet population by using a number density function (NDF), which satisfies a population balance equation (PBE), also called Williams-Boltzmann Equation (WBE) [10]. Kah et al. [11] derived from this equation a high order moment method called Eulerian Multi-Size Moment model (EMSM), which tackles the modeling and numerical simulation of polydisperse sprays flows in a monokinetic configuration. In the EMSM model, the size distribution is described through a set of high order size-moments. Anytime, the size distribution can be reconstructed from this set by using an Entropy Maximization technique, thus providing the model with a natural closure.

In order to design a model which could be also used further upstream, *i.e.* closer to the injector, we will rely in the present work on the same idea of deriving a system of conservation equations on a set of high order size moments, except that we will use another set of moments, which can be identified as averaged geo-

metrical information of the interface between the two phases. In fact, the interfacial geometry has a major effect on the dynamics of interfacial flows and an accurate geometrical description of this phase is mandatory. The key issue is then to be able to construct a set of high order moments, which can both describe some level of topological information about the averaged interface and allow to reconstruct a size distribution in the spray region, and therefore deal with evaporation and other spray-gas exchange terms. For this purpose, we introduce a new model, where the geometrical variables are expressed as fractional size-moments.

Whereas the mathematical aspects of such an approach are tackled in [12] (structure of the moment space, treatment of the frontiers of the moment space, realizability conditions...), we focus here on introducing the model with an engineering point of view, for the sake of clarity. As in [4], we stay in a simplified framework, but nonetheless provide more details on the link with averaged model for interfacial flows. This is the first novelty of the paper. Next, a dedicated numerical treatment to transport the resulting model in physical and phase space (such as evaporation) is briefly presented. This numerical method always guarantees the realizability of the set of transported moments. We refer to [12] for detailed numerical analysis. Finally, the whole method has been implemented in a code, called `CanOP` [13, 4]. In order to deal with adaptive mesh refinement, which will be essential in many two-phase flow configurations, as well as with massively parallel architecture, this code is based on the `p4est` library [3]. The efficiency of the code is investigated in [4]. Here, we will rather focus on the physics and study a difficult case, as far as mesh refinement is concerned. This configuration is a homogeneous isotropic turbulence, laden with polydisperse particles. The model and the numerical method are assessed through comparisons with a Lagrangian approach and this will allow us to show the potential of the proposed approach.

The paper is organized as follows. In the second section, we present the general framework of spray modeling at mesoscopic scale and then we briefly recall the fundamentals of Kah et al [1] we will rely on. In the third section, we present the motivation and the importance of using geometrical modeling of the interface and introduce the new topological moment model. In the fourth section, we show the ability of this new Eulerian model to predict the disperse phase segregation in a turbulent gaseous carrier flow, using adaptive mesh refinement grid for high resolution and low computational cost.

## 2. Spray modeling

The spray consists in a cloud of polydisperse droplets interacting with the surrounding gas and possibly with each other. In the present work, we consider dilute sprays of small droplets such that the coalescence and secondary break-up can be neglected. In the following, we present the Eulerian moment model derived from a statistical approach. First, let us introduce the number density function (NDF)  $f(t, \vec{x}, \vec{c}, S)$ , which represents the probable number of droplets located at position  $\vec{x}$ , travelling with velocity  $\vec{c}$  and having size  $S$ . If not specified otherwise,  $S$  is a surface. At the mesoscopic scale, the NDF satisfies a WBE<sup>1</sup> [10]. In the following, we use a dimensionless formulation of this equation:

$$\partial_t f + \partial_{\vec{x}} \cdot (\vec{c} f) + \partial_{\vec{c}} \cdot \left( \frac{\vec{u}_g - \vec{c}}{\text{St}(S)} f \right) + \partial_S (R_S f) = 0, \quad (1)$$

where  $\frac{\vec{u}_g - \vec{c}}{\text{St}(S)}$  is the drag force given by Stokes law, under the assumption of low Reynolds number,  $\vec{u}_g$  is the gas velocity,  $\text{St}$  is the Stokes number which is supposed to depend linearly on the surface of the droplets  $\text{St}(S) = \theta S$  and  $R_S(S) = \frac{dS}{dt}$  is the

evaporation rate. We consider the case of a  $d^2$  evaporation law, thus, the evaporation rate is constant:  $R_S = -K < 0$ .

Next, we reduce this kinetic model to a system of conservation laws by solving for the first moments of the NDF. The velocity-size moment is defined by:

$$M_{i,j,k,l} = \int_0^{S_{max}} \int_{\mathbb{R}^3} S^l v_x^i v_y^j v_z^k f(t, \vec{x}, \vec{v}, S) dS d^3 \vec{v}, \quad (2)$$

where the maximum size  $S_{max}$  can be set to 1 since we use dimensionless variables. In the following, we consider a monokinetic-equilibrium assumption [14, 15], where all the droplets at a given position and time have the same velocity. Moreover this velocity is assumed not to depend on the droplet size for the sake of simplicity. We refer to [16] for a size-velocity correlation resolution. Therefore, the distribution velocity is given by the following Dirac delta distribution:

$$f(t, \vec{x}, \vec{c}, S) = n(t, \vec{x}, S) \delta(\vec{c} - \vec{u}(t, \vec{x})), \quad (3)$$

where  $n(t, \vec{x}, S)$  is the size distribution and  $\vec{u}(t, \vec{x})$  is the macroscopic velocity. Kah derived the EMSM model [11] as the dynamics of the successive  $N$  size-moments of the WB equation:

$$\begin{aligned} \partial_t m_0 + \partial_{\vec{x}} \cdot (m_0 \vec{u}) &= -n(S=0), \\ \partial_t m_1 + \partial_{\vec{x}} \cdot (m_1 \vec{u}) &= -K m_0, \\ \partial_t m_2 + \partial_{\vec{x}} \cdot (m_2 \vec{u}) &= -2K m_1, \\ &\vdots \\ \partial_t m_N + \partial_{\vec{x}} \cdot (m_N \vec{u}) &= -NK m_{N-1}, \\ \partial_t (m_1 \vec{u}) + \partial_{\vec{x}} \cdot (m_1 \vec{u} \otimes \vec{u}) &= -K m_0 \vec{u} + m_0 \frac{\vec{u}_g - \vec{u}}{\theta}, \end{aligned} \quad (4)$$

where  $m_k = \int_0^1 S^k n(t, \vec{x}, S) dS$  is the  $k^{\text{th}}$  order size-moment. In order to close the system, Massot et al [17] proposed to reconstruct the size distribution by maximizing Shannon entropy:

$$H(n) = - \int_0^1 n(s) \ln(n(s)) ds. \quad (5)$$

The existence and uniqueness of a function density  $n$  which maximizes the Shannon entropy and satisfies:

$$\begin{aligned} m_0 &= \int_0^1 n(S) dS, \\ &\vdots \\ m_N &= \int_0^1 S^N n(S) dS, \end{aligned} \quad (6)$$

were proved in [18]. The solution has the following form:

$$n(S) = \exp \left( -(\lambda_0 + \lambda_1 S + \dots + \lambda_N S^N) \right). \quad (7)$$

This model shows a great capacity to describe the polydisperse character of the spray in an Eulerian modeling framework [16], especially for automotive engines [19]. Even if the use of an Eulerian framework makes the coupling easier with the other reduced order model near the injector, which is usually a diffuse interface model, Eulerian as well, this coupling still encounters several difficulties and remains an open problem. Then, we need a way of describing the polydisperse spray through a high order size moment approach, which could be related to the geometrical properties of the interface. This is the purpose of next section.

<sup>1</sup>We directly work in a simplified framework and notice that the extension of the approach to more complex droplet models can be conducted without problem [2].

### 3. High order geometrical size moment for polydisperse evaporating sprays - relation with interface average topology

The final droplets size distribution downstream the injection device depends widely on the flow close to injector. There, the liquid fuel is injected at high speed and pressure and the interaction with the surrounding gas is located at a very thin interface. In this first region, the two phases are considered as separated phases and the dynamics of the interface will have a major influence on the atomization process and thus, on the formation of the polydisperse spray.

In fact, the exchange of mass, momentum and energy between both phases depend on the interface area. Besides, after the interface has been destabilized through aerodynamics forces, a region of high complexity is to be found where ligaments are formed and disintegrate into droplets of various sizes. These droplets can even experience secondary break-up and coalescence and the whole process yields a very large spectrum of scales in terms of interface dynamics. The exact location of each phase is difficult to determine because of different chaotic phenomena such as turbulence, interface instabilities and other small scale phenomena that cannot be simulated even with the most powerful calculators. Fortunately, industrial applications are more concerned with the main features of the flow than with its small details. Thus, only averaged quantities can be resolved and we can use diffuse interface models (DIM) [20, 21, 22]. The derivation of the DIM is based on some averaging-like operator (ensemble-average, time-average or volume-average). By considering some equilibrium assumptions, a hierarchy of models can then be derived. In this approach, the interface is considered as a mixing zone, such that the two phases coexist at the same macroscopic position, and each phase occupies a fraction of the volume. The derivation of the model is based on averaging methods [23] applied to the monophasic Navier-Stokes equations of each phase. This way, we obtain a set of equations which involves the volume fraction function. This variable takes values close to 1 in regions of a pure given phase and values close to 0 in the regions where this phase nearly disappears. Crossing the interface, the volume fraction varies continuously from 0 to 1 or the other way around. Thereby, the interface is considered as a narrow layer instead of a sharp discontinuity. This assumption smoothes out the small variations and details of the interface. As a result, some geometrical information about the interface are lost, what could be interpreted as ignoring the small scale effects. One has then to find a way to enrich the model with geometrical information about the interface.

#### 3.1. Drew's model for geometrical averaged quantities

In order to correct this default, Drew [24] proposed an accurate description for the interface dynamics, based on considering some geometrical variables, which satisfy kinematic equations for the rate of change of the volume fraction, interface area density, and curvature variables. In the following, we present the geometrical variables in the context of a general separated phases two-phase flow. The details of the resulting transport equations are not presented for the sake of clarity and the readers can refer to the article [24]. The important point is to focus on the proper set of geometrical variables, which have some physical meaning and, which will be identified in the specific framework of a polydisperse spray.

In the following, we define some average geometrical variables that can be used to model the interface between separated phases. Their definition is based on the volume-average operator. First, we define the phase function  $\chi_k(t, \vec{x})$  for a given phase  $k$  by:

$$\chi_k(t, \vec{x}) = \begin{cases} 1, & \text{if } \vec{x} \in k \\ 0, & \text{otherwise.} \end{cases}$$

Next, the volume-average operator is defined by:

$$\overline{(\bullet)}(t, \vec{x}) = \frac{1}{|V|} \int_V (\bullet) \chi_k(t, \vec{x}) dV(\vec{x}), \quad (8)$$

where  $V \in \mathbb{R}^3$  is a macroscopic neighborhood of position  $\vec{x}$ , and  $|V|$  its volume.

Let us emphasize that the averaged set of conservation equations of is obtained by applying this operator to the monophasic Navier-Stokes equations. The obtained equations involve the volume fraction variable, which expresses the fraction of volume occupied by a given phase. Moreover, this variable allows to locate the interface up to the averaging scale and is then a first piece of information about the interface geometry [1]. It writes:

$$\alpha_k(t, \vec{x}) = \frac{1}{|V|} \int_V \chi_k(t, \vec{x}) dV(\vec{x}). \quad (9)$$

In order to model exchange terms, such as evaporation, thermal transfer and drag force, Drew [24] or other two-phase flows models [25, 26, 8] consider an additional topological variable: the interfacial area density. It can be interpreted as the ratio of the interface area present in a macroscopic neighborhood to its volume. This variable can be written as the volume-average of the norm of the gradient of the phase function  $\chi_k$ :

$$\Sigma(t, \vec{x}) = \frac{1}{|V|} \int_V \|\vec{\nabla} \chi_k(t, \vec{x})\| dV(\vec{x}). \quad (10)$$

So far, the interface modeling is still incomplete, since no information on the interface shape is available. In fact, the small details of the interface can not be modeled accurately using only two geometrical variables. Drew proposed to introduce the two principal curvatures of the interface in his model. Indeed, these variables give a complementary description of the interface and are highly related to the atomization process, since they are involved in the jump relations at the interface.

The two local principal curvatures are defined as follows: we consider a point  $P$  at the interface and the associated normal vector  $\vec{n}$ . Then, we take a plane that contains  $P$  and  $\vec{n}$  and let it rotate around the normal. For each position of this plane, the intersection curve between the interface and the rotated plane defines a curvature at point  $P$  which corresponds to the curvature of this manifold. As the plane completes a full  $\pi$  rotation, it reaches exactly two extremal curvature values: the two principal curvatures  $k_1$  and  $k_2$ .

Then, Drew derived the equation of the dynamics of the mean and of the Gauss curvature from the differential equations ruling  $k_1$  and  $k_2$ . The mean curvature  $H$  and the Gauss curvature  $G$  are defined by:

$$\begin{aligned} H &= \frac{1}{2}(k_1 + k_2), \\ G &= k_1 k_2. \end{aligned} \quad (11)$$

Since these interfacial variables are properly defined only at the interface, they need a specific operator to be averaged. We introduce the interface-average operator  $\widetilde{\Sigma}(\bullet)$ , defined as:

$$\widetilde{\Sigma}_k(\bullet)(t, \vec{x}) = \frac{1}{|V|} \int_V (\bullet) \|\vec{\nabla} \chi_k(t, \vec{x})\| dV(\vec{x}). \quad (12)$$

The interface-averaged Gauss and mean curvature weighted by the interface density are defined as follows :

$$\begin{aligned} \widetilde{\Sigma H} &= \int_V H \|\vec{\nabla} \chi_k(t, \vec{x})\| dV(\vec{x}), \\ \widetilde{\Sigma G} &= \int_V G \|\vec{\nabla} \chi_k(t, \vec{x})\| dV(\vec{x}). \end{aligned} \quad (13)$$

### 3.2. High order geometrical moments for a polydisperse spray

Finally, we derive from the kinetic model a new high order size moment model describing the interfacial geometry evolution at the scale of a polydisperse and monokinetic spray, using the previously defined variables. In the disperse phase, droplets are of spherical shape. Therefore, they involve various level of curvature and interface area depending on their size. However, considering a population of droplets, we can describe the mean topological geometry of the ensemble by analogy with interfacial flow. Considering the interface description given in the last section, we transport the same geometrical variables.

Above, the definition of the geometrical variables (volume fraction, interfacial area density, mean and Gauss curvature) have been defined based on the phase function  $\chi_k$ . This function contains all the microscopic information about the interface. In the context a polydisperse spray, we use the statistical information about the droplet distribution, which is given by the size distribution  $n(t, \vec{x}, S)$ . Considering this function, we define the various geometrical variables in the context of a polydisperse spray.

- The *volume fraction*  $\alpha_d$  is the sum of the volume of each droplet divided by the containing volume at a given position:

$$\alpha_d = \int_0^1 V(S)n(t, \vec{x}, S)dS. \quad (14)$$

The droplet being spherical,  $V(S) = \frac{S^{3/2}}{6\sqrt{\pi}}$ .

- The *interfacial area density*  $\Sigma_d$  is the sum of the surface of each droplet divided by the containing volume at a given position:

$$\Sigma_d = \int_0^1 S n(t, \vec{x}, S)dS. \quad (15)$$

- The two local curvature radii are equal for spherical droplets  $R_1 = R_2 = \frac{\sqrt{S}}{2\sqrt{\pi}}$ . But, since we use the mean and Gauss curvatures, two different averaged quantities can be defined. This can also justify the use of Gauss and mean curvatures instead of considering directly the two principal curvatures. Let us notice that, in the case of separated phases, the *average mean and Gauss curvatures* have been defined as an average over a volume and weighed by the interfacial area. In the disperse phase case, this becomes:

$$\begin{aligned} \Sigma_d \tilde{H}_d &= \int_0^1 H(S) S n(t, \vec{x}, S) dS, \\ \Sigma_d \tilde{G}_d &= \int_0^1 G(S) S n(t, \vec{x}, S) dS. \end{aligned} \quad (16)$$

Finally, these four geometrical variables can be expressed as fractional moments of the NDF:

$$\begin{aligned} \Sigma_d \tilde{G}_d &= 4\pi m_0, \\ \Sigma_d \tilde{H}_d &= 2\sqrt{\pi} m_{1/2}, \\ \Sigma_d &= m_1, \\ \alpha_d &= \frac{1}{6\sqrt{\pi}} m_{3/2}, \end{aligned} \quad (17)$$

where the half-integer moments are defined by

$$m_{k/2} = \int_0^1 S^{k/2} n(S) dS. \quad (18)$$

In fact, these moments could be expressed as integer moments by simple variable substitution  $R = \sqrt{S}$ . However, we prefer to hold with the droplet surface as the size variable, since

we consider a  $d^2$  evaporation law, for which the evaporation rate  $R_s = dS/dt$  is constant.

Following the same derivation as the EMSM model, we derive the following system of conservations laws for the new moments:

$$\begin{cases} \partial_t m_0 + \partial_{\vec{x}} \cdot (m_0 \vec{u}) &= -n(t, S=0) \\ \partial_t m_{1/2} + \partial_{\vec{x}} \cdot (m_{1/2} \vec{u}) &= -\frac{K}{2} m_{-1/2} \\ \partial_t m_1 + \partial_{\vec{x}} \cdot (m_1 \vec{u}) &= -K m_0 \\ \partial_t m_{3/2} + \partial_{\vec{x}} \cdot (m_{3/2} \vec{u}) &= -\frac{3K}{2} m_{1/2} \\ \partial_t (m_1 \vec{u}) + \partial_{\vec{x}} \cdot (m_1 \vec{u} \otimes \vec{u}) &= -K m_0 \vec{u} + m_0 \frac{\vec{u}_g - \vec{u}}{\theta} \end{cases} \quad (19)$$

where  $K$  is the constant evaporation rate for the  $d^2$  evaporation law.

By analogy with the EMSM model, from a set of moments, we reconstruct the continuous distribution  $n(t, \vec{x}, S)$  by entropy maximization, what allows us to close the system. The existence and uniqueness of such a reconstruction, as well as the behavior at the frontier of the moment space have been studied in [12]. Also, it is shown that the reconstructed NDF has the following form:

$$n^{EM}(S) = \exp\left(-(\lambda_0 + \lambda_1 S^{1/2} + \lambda_2 S + \lambda_3 S^{3/2})\right). \quad (20)$$

The  $\lambda_i$  coefficients are determined thanks to the same inversion algorithm as in [18]: a convex optimization under constraints.

Let us emphasize that this model can be extended to a hybrid method between high order moment method and Multi-Fluid model, by considering multiple size intervals, called sections. In our case, exchange terms between sections due to evaporation have to be considered. Nevertheless, these new terms do not introduce any further difficulty compared to the one section case and the multi-section case can be treated the same way [12, 16].

## 4. Results

This model has been implemented in the `CanOP` code [13, 4]. It is a C/C++ Code developed for multi-applications, based on finite volume solvers and relying on the adaptive mesh refinement library `p4est` [3]. The resolution of the system (19) is done using operator splitting techniques [14, 15], what allows us to separate the resolution of the two main phenomena, transport in physical space (solving for a system of conservation laws) and transport in phase space through source terms (evaporation and drag force), thus leading to a very efficient algorithm on parallel architectures, when coupled to adaptive mesh refinement [4]<sup>2</sup>. The transport in physical space relies on a finite volume schemes of order two for non-conforming meshes [4], whereas a new evaporation algorithm has been developed in [12]. The whole numerical process allows for a fully realizable scheme: it guarantees that the vector of moments always remains within the space of moments.

$Re_t$	$\epsilon$	$\eta_k$	$\tau_k$	$TKE$
25	$1e-3$	$3.2e-2$	1.	$1.e-2$

Table 1: Turbulence properties of the 3D HIT gaseous flow field

As a complement to the studies conducted in [4, 12], we assess the capability of the proposed approach by investigating a 3D configuration of a non-evaporating spray in the presence of a frozen Homogeneous Isotropic Turbulence flow (HIT). The HIT gaseous flow field has been generated independently by Sabat [27] with the ASPHODELE code of CORIA [28], which solves the three-dimensional Navier-Stokes equations for the gas phase

<sup>2</sup>A detailed studies to assess the robustness and accuracy of the numerical scheme as well as the parallel performance of `CanOP` code can be found in [4, 12].

in the low-Mach number limit. The characteristics of this HIT is given in Table 4, where  $Re_t$  is the turbulent Reynolds number,  $\epsilon$  is the mean dissipation rate,  $\eta_k$  is the smallest structures size,  $\tau_k$  is the Kolmogorov time scale of the turbulence, and  $TKE$  is the turbulent kinetic energy. The mean Stokes number of the polydisperse spray is taken as  $St = 0.5$

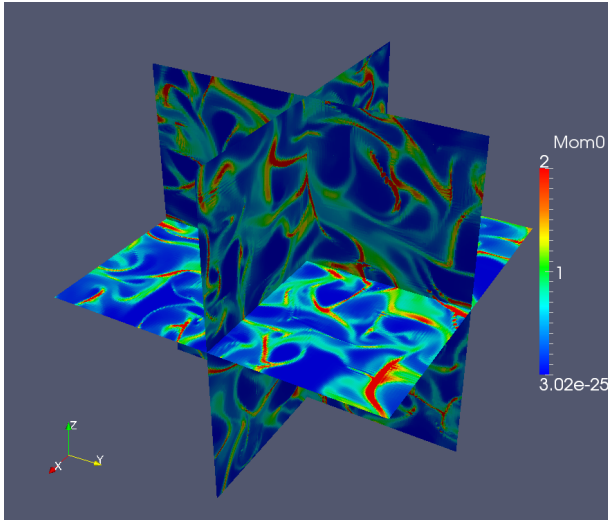


Figure 1: Number density of the droplets given by the moment  $m_0$ , on an AMR grid at  $t = 12$ .

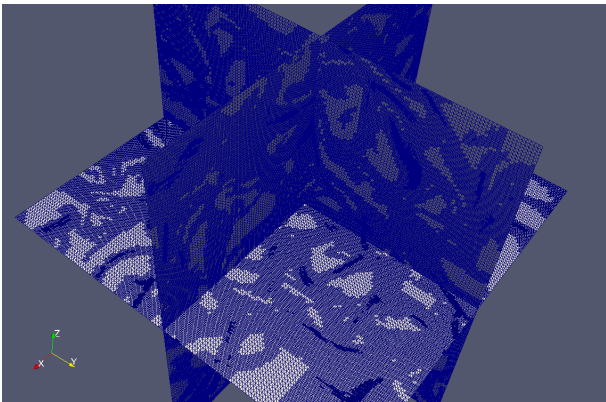


Figure 2: The AMR grid at  $t = 12$ .

The simulation is performed with an adaptive mesh, where the maximum and minimum refinement levels,  $l_{max} = 9$  and  $l_{min} = 7$ , correspond respectively to a mesh of size  $\delta x_{min} = 2^{-9}$  and  $\delta x_{max} = 2^{-7}$  for a dimensionless grid  $[0, 1]^3$  (the real physical domain dimension is  $5m \times 5m \times 5m$ ). The refinement criterion is based on an heuristic estimation of the  $L^1$ -norm of the error and requires a thorough study of the threshold influence on the solution quality [4]. In Figure 1, we display a three cut sections of the spray density, as well as the corresponding mesh in Figure 2. The first figure shows the segregation of the spray in low vorticity regions. For the present choice of refinement criterion, the compression rate is 91.56%. In Figure 3, we compare the segregation evolution obtained in this Eulerian simulation with a Lagrangian result (see [27]). The segregation is

computed using the spray moment  $m_0$  as follows:

$$\frac{\langle (m_0)^2 \rangle}{\langle m_0 \rangle^2} \quad \text{where} \quad \langle \bullet \rangle = \frac{1}{V} \int_V \bullet \, dV.$$

We can see that in the AMR Eulerian simulation, we make a small error on predicting the segregation compared to the Lagrangian simulation because of the numerical diffusion and eventually the monokinetic-equilibrium assumption. A detailed study conducted in [27] shows that the produced results stays very closely comparable to the monokinetic Eulerian results on the finest grid, which exhibit the same small difference based on numerical diffusion and modeling assumptions for this range of Stokes numbers.

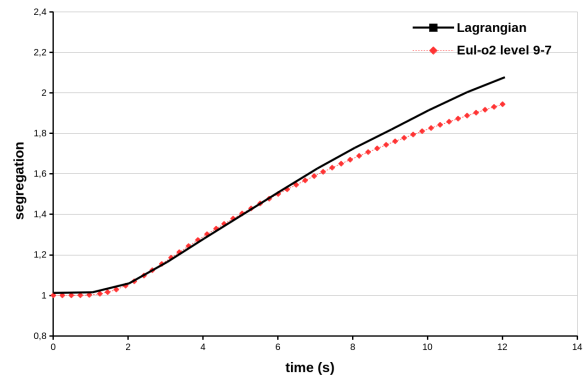


Figure 3: Evolution of the segregation with time for the Lagrangian simulation (black solid line) and our Eulerian model with AMR (red dotted line).

## 5. Conclusion

In this paper, we have introduced a new geometrical high order size moment method, which allows both to capture the dynamics of a polydisperse evaporating spray and to make the link with physically relevant interfacial geometrical quantities. It should help designing a unified model able to resolve the full spectrum of scales, from the injector mouth down to the polydisperse spray region, via the region where the atomization process occurs. Also, the dedicated numerical scheme developed in this context [12, 4] is proven to be accurate, robust and realizable.

The second contribution of this paper consists in using adaptive mesh refinement, in order to reach a fine mesh resolution in the high concentrated zones, while keeping low resolution in other emptying regions, and thus gaining computational cost. Finally, the validity of the whole modeling and numerical process is assessed by looking at the evolution of the segregation in a homogeneous isotropic turbulence laden with a polydisperse spray. The comparison with a reference Lagrangian simulation is very satisfying.

Let us underline that for the moment, we have focused only on a rather simple modeling level and used only one single section to describe the polydisperse spray. Using the ideas developed in [16], size-conditioned dynamics should be easily taken into account by using more size sections. Also, the monokinetic-equilibrium assumption could be relaxed and hydrodynamical equilibrium velocity distribution could be considered. However, this would involve higher order velocity moments [27] and a diffuse interface model involving such quantities still has to be designed. This is work in progress.

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## References

- [1] D. Kah, *Taking into account polydispersity in the framework of a coupled Euler-Lagrange approach for the modeling of liquid fuel injection in internal combustion engines*. PhD thesis, Ecole Centrale de Paris, 2010. available online at <http://tel.archives-ouvertes.fr/tel-00618786/en/>.
- [2] O. Emre, *Modeling of spray polydispersion with two-way turbulent interactions for high pressure direct injection in engines*. PhD thesis, Ecole Centrale Paris, 2014. Available at <https://tel.archives-ouvertes.fr/tel-01089937>.
- [3] C. Burstedde, L. C. Wilcox, and O. Ghattas, “p4est: Scalable algorithms for parallel adaptive mesh refinement on forests of octrees,” *SIAM Journal on Scientific Computing*, vol. 33, no. 3, pp. 1103–1133, 2011.
- [4] M. Essadki, S. de Chaisemartin, M. Massot, F. Laurent, A. Larat, and S. Jay, “High order moment methods and adaptive mesh refinement for polydisperse evaporating spray simulations,” *Submitted to Oil & Gas Science and Technology*, 2016.
- [5] C. Hirt, A. Amsden, and J. Cook, “An arbitrary lagrangian-eulerian computing method for all flow speeds,” *Journal of Computational Physics*, vol. 14, no. 3, pp. 227–253, 1974.
- [6] F. Harlow and J. E. Welch, “Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface,” *The physics of Fluid*, vol. 8, no. 12, pp. 2182–2189, 1965.
- [7] T. Menard, S. Tanguy, and A. Berlemont, “Coupling level set/VOF/ghost fluid methods: Validation and application to 3D simulation of the primary break-up of a liquid jet,” *International Journal of Multiphase Flow*, vol. 33, no. 5, pp. 510–524, 2007.
- [8] R. Lebas, T. Menard, P. A. Beau, A. Berlemont, and F. X. Demoulin, “Numerical simulation of primary break-up and atomization: DNS and modelling study,” *Int. J. Multiphase Flows*, vol. 35, no. 3, pp. 247–260, 2009.
- [9] V. L. Chenadec and H. Pitsch, “A 3D unsplit forward/backward volume-of-fluid approach and coupling to the level set method,” *Journal of Computational Physics*, vol. 233, no. 0, pp. 10 – 33, 2013.
- [10] F. Williams, “Spray combustion and atomization,” *Physics of Fluids*, vol. 1, pp. 541–545, 1958.
- [11] D. Kah, F. Laurent, M. Massot, and S. Jay, “A high order moment method simulating evaporation and advection of a polydisperse spray,” *J. Comput. Phys.*, vol. 231, no. 2, pp. 394–422, 2012.
- [12] M. Essadki, S. de Chaisemartin, F. Laurent, A. Larat, and M. Massot, “Topological moment model for polydisperse evaporating sprays,” *Submitted to SIAM Journal on Applied Mathematics*, 2016.
- [13] F. Drui, A. Fikl, P. Kestener, S. Kokh, A. Larat, V. Le Chenadec, and M. Massot, “Experimenting with the p4est library for AMR simulations of two-phase flows,” *to appear in ESAIM : Proceedings and Surveys*, pp. 1–16, 2016.
- [14] S. de Chaisemartin, L. Fréret, D. Kah, F. Laurent, R. Fox, J. Reveillon, and M. Massot, “Eulerian models for turbulent spray combustion with polydispersity and droplet crossing,” *Comptes Rendus Mécanique*, vol. 337, pp. 438–448, 2009. Special Issue ‘Combustion for Aerospace Propulsion’.
- [15] S. de Chaisemartin, *Eulerian models and numerical simulation of turbulent dispersion for polydisperse evaporation sprays*. PhD thesis, Ecole Centrale Paris, France, 2009. Available on TEL : <http://tel.archives-ouvertes.fr/tel-00443982/en/>.
- [16] A. Vié, F. Laurent, and M. Massot, “Size-velocity correlations in high order moment methods for polydisperse evaporating sprays: modeling and numerical issues,” *J. Comp. Phys.*, vol. 237, pp. 277–310, 2013.
- [17] M. Massot, F. Laurent, D. Kah, and S. de Chaisemartin, “A robust moment method for evaluation of the disappearance rate of evaporating sprays,” *SIAM J. Appl. Math.*, vol. 70, pp. 3203–3234, 2010.
- [18] L. R. Mead and N. Papanicolaou, “Maximum entropy in the problem of moments,” *J. Math. Phys.*, vol. 25, no. 8, pp. 2404–2417, 1984.
- [19] D. Kah, O. Emre, Q. Tran, S. de Chaisemartin, S. Jay, F. Laurent, and M. Massot, “High order moment method for polydisperse evaporating spray with mesh movement: application to internal combustion engines,” *International Journal of Multiphase Flows*, vol. 71, pp. 38–65, 2015.
- [20] M. R. Baer and J. W. Nunziato, “A two-phase mixture theory for the deflagration-to-detonation transition (DDT) in reactive granular materials,” *International Journal of Multiphase Flow*, vol. 12, no. 6, pp. 861–889, 1986.
- [21] R. Saurel and R. Abgrall, “A multiphase godunov method for compressible multifluid and multiphase flows,” *Journal of Computational Physics*, vol. 150, no. 2, pp. 425 – 467, 1999.
- [22] R. Saurel and O. Lemetayer, “A multiphase model for compressible flows with interfaces, shocks, detonation waves and cavitation,” *Journal of Fluid Mechanics*, vol. 431, no. 2, pp. 239–271, 2001.
- [23] D. Drew and S. Passman, “Theory of multicomponent fluids,” 1999.
- [24] D. A. Drew, “Evolution of geometric statistics,” *SIAM J. Appl. Math.*, vol. 50, no. 3, p. 649–666, 1990.
- [25] A. Vallet, A. Burluka, and R. Borghi, “Development of a eulerian model for the “atomization” of a liquid jet,” *Atomization and Sprays*, vol. 11, pp. 619–642, 2001.
- [26] S. Jay, F. Lacas, and S. Candel, “Combined surface density concepts for dense spray combustion,” *Combustion and Flame*, vol. 144, no. 3, pp. 558–577, 2006.
- [27] M. Sabat, *Modèles Eulériens et méthodes numériques pour la description des sprays polydispersés turbulents*. PhD thesis, Université Paris-Saclay, CentraleSupélec, 2016.
- [28] J. Reveillon and F. Demoulin, “Effects of the preferential segregation of droplets on evaporation and turbulent mixing,” *Journal of Fluid Mechanics*, vol. 583, pp. 273–302, 2007.