Modeling of polydisperse sprays using a high order size moment method for the numerical simulation of advection and evaporation

D. Kah[*,**,§], F. Laurent[*], M. Massot[*], S. Jay[**]
[*] Laboratoire EM2C, UPR CNRS 288, Ecole Centrale Paris
Grande Voie des Vignes
92295 CHATENAY-MALABRY, FRANCE
[**] Institut Français du Pétrole
1 & 4 Avenue de Bois Préau
92852 RUEIL MALMAISON, FRANCE

Abstract

This article investigates the critical issue of stable Eulerian high order size moment methods in the numerical modeling of polydisperse evaporating sprays. Polydispersity has to be modeled in order to reproduce the physics of dispersion and evaporation in most practical devices. Eulerian size moment methods are well suited for such problems but the design of numerical algorithms usually faces two difficulties: numerical diffusion and stability. The vector of successive size moments of a number density function (NDF) over a given size interval belongs to what is called the moment space, the geometry of which is complex. Any numerical method has to preserve this property and it has been shown to be a critical issue in the literature. In this paper we use a high order size moment method and design a new numerical scheme for transport in physical space, which is shown to be second order in both time and space and provides stability in the sense that it allows to preserve the ground property of a size moment vector, that is, to belong to the moment space. We also introduce operator splitting techniques and show how this new algorithm can be coupled to an evaporation module which models the disappearing droplet flux with high precision and also preserve the moment space [7]. Such an accurate and stable scheme able to transport and evaporate a polydisperse particle/droplet flow might be of great interest for all applications where the knowledge of the size distribution of a population is an issue, in particular for engine spray applications.

Introduction

The accurate simulation of multiphase flow has become a crucial issue since it is involved in a lot of industrial applications such as combustion, chemical engineering science, biology, biochemistry, air quality and climate change studies. The background of our work is the study of a dilute droplet cloud with a relatively small volume fraction $\alpha<10^{-2}$, in a gaseous carrier flow; this cloud is usually polydisperse, i.e. it contains a large particle size distribution (PSD). This is typical of a fuel jet downstream an injector after the breakage process in internal combustion engines.

The modeling of the dispersed liquid phase relies on a kinetic description at a mesoscopic level called the Williams' equation on the number density function f for which size appears as one dimension of the phase space

$$\partial_t f + \partial_x (\boldsymbol{v} f) + \partial_S (Rf) + \partial_v (F/m\, f) + \partial_T (Ef) = \Gamma \qquad (1)$$

This approach describes the droplet as a cloud of point particles which experience transport in real space with velocity $\boldsymbol{v}$, droplet evaporation with evaporating rate R, acceleration of droplets due to drag F/m, heat exchange the rate of which is E, and coalescence-breakup of droplets through Γ. As the flow is assumed to be dilute and the particles small enough, collisions can be neglected in the limit of large Knudsen number. For the purpose of demonstrating the ability of our method and for the sake of legibility, we will restrict the investigation to the configuration where only advection and evaporation are taken into account and we only consider the first three terms of Eq (1)

$$\partial_t f + \partial_x (\boldsymbol{v} f) + \partial_S (Rf) = 0 \qquad (2)$$

All the conclusions drawn from this study can easily be extended to heat and drag. A deterministic Direct Numerical Simulation of Eq. (2) is intractable. Thus we investigate a Eulerian method of moments (MOM) in order to solve Eq. (1) even if we loose some information on f (see [8,9] and references therein). A paramount characteristic of the

[§]Damien Kah: damien.kah@em2c.ecp.fr, damien.kah@ifp.fr

droplet phase that has to be modeled in order to have accurate simulations is its polydispersity because it strongly impacts on the coupling terms between the two phases. Once a closure has been chosen in terms of velocity moments conditioned in droplet size [3,6], there are basically two options in order to capture the dynamics in the size phase space. One can either rely on a size phase space discretization with low order size moments in each section such as in the multi-fluid approach developed by some of the authors in [2,3,6] from [5], or consider only one size interval and introduce high order size moments. The multi-fluid model only considers one moment size accounting for the liquid mass on small intervals of the size phase space called sections has been shown to yield simple transport algorithms for transport in physical space in [2,3] easily implemented on parallel architectures; however, the cost of the discretization in size phase space is high and the possibility of a high order moment method is very attractive in terms of computational cost and in the context of extending such an approach to a two-fluid model.

We thus focus this study on high order size moment methods in the context of transport in physical space and evaporation. When it comes to pure advection, the corresponding system is closed. But one faces great difficulties to design a numerical scheme with low numerical diffusion, i.e. at least 2nd order in space. Indeed, algorithms which transport the moments as independent tracers generate invalid moment sets, that is moments which are out of the moment space and for which no NDF can be found such that they are the moments this NDF. Some interesting transport algorithms have been devised in [8] and [9] for which the preservation of the moment space can be attained through additional projections. The algorithm is not able *per se* to preserve the moment space and lacks stability.

In this paper, we propose a numerical 2nd order scheme, which preserves the moment space without any additional projection algorithm. The innovative and ground idea of our work is to consider transported quantities belonging to a space whose geometry is much easier to deal with, so that they can be easily controlled. These quantities are called canonical moments. After introducing the set of conservation laws satisfied by the moments as well as the theoretical tools needed, we introduce the new algorithm and provide an example proving its efficiency. We then show how our new approach can be easily coupled through operator splitting to another algorithm introduced in [7], which has the ability to treat evaporation and to preserve the moment space. Its main features are recalled and a second test-case displays the ability of the our approach to finally fully treat evaporation and transport in physical space in 2D.

Model for the advection of size moments

We start with Eq. (2) with no evaporation and consider the NDF $f(t,\boldsymbol{x},S,\boldsymbol{v})$, where $\boldsymbol{x}$ is space, $\boldsymbol{v}$ is velocity and S the surface, which accounts for size as we consider spherical droplets which satisfies the "kinetic" equation:

$$\partial_t f + \partial_{\boldsymbol{x}}(\boldsymbol{v}f) = 0 \qquad (3)$$

In order to close the system on the velocity moments of order zero and one and obtain the semi-kinetic system as in [3,6], we assume that the velocity dispersion at fixed size is null, which is legitimate as we consider laminar flows or Direct Numerical Simulation configurations. Therefore we project f on a distribution with a single velocity conditioned by size. So f is presumed as $f(t,\boldsymbol{x},S,\boldsymbol{v}) = n(t,\boldsymbol{x},S)\delta(\boldsymbol{v} - \boldsymbol{u}(t,\boldsymbol{x},S))$ and the system on n and $\boldsymbol{u}$ reads:

$$\begin{aligned} &\partial_t n + \partial_{\boldsymbol{x}}(n\boldsymbol{u}) = 0 \\ &\partial_t n\boldsymbol{u} + \partial_{\boldsymbol{x}}(n\boldsymbol{u}\otimes\boldsymbol{u}) = 0 \end{aligned} \qquad (4)$$

From there, we further assume that the velocity $\boldsymbol{u}$ does not depend on droplet size, as it is the case for non-inertial droplets or particles which are advected by the gaseous velocity field and take the successive integer moments in terms of surface of system (4). Up to a non-dimensional form of the equations, we can assume that the system in in non-dimensional form and that the size interval is [0,1]. This leads to a system of conservation equations on moments $m_k = \int_0^1 S^k n(t,\boldsymbol{x},S)dS$ of order *0* to *N*. In this paper, we will consider *N=3*, which is a good compromise between accuracy and computational cost. A detailed study of the moment space geometry provided in [7] illustrates why this choice is a accurate enough for evaporation and convection. The resulting system writes:

$$\begin{aligned} &\partial_t m_0 + \partial_{\boldsymbol{x}}(m_0\boldsymbol{u}) = 0 \\ &\qquad\vdots \\ &\partial_t m_3 + \partial_{\boldsymbol{x}}(m_3\boldsymbol{u}) = 0 \\ &\partial_t m_0\boldsymbol{u} + \partial_{\boldsymbol{x}}(m_0\boldsymbol{u}\otimes\boldsymbol{u}) = 0 \end{aligned} \qquad (5)$$

Moment space, canonical moments and pressureless gas dynamics

The main difficulty with system (5) is to make sure that the vector $(m_0,\ldots,m_N)^t$ can always be related to a NDF *f*, so that $\int_0^1 S^k f(S)dS = m_k$. Vectors verifying this condition belong to the moment space of order *N*, M_N. But not all the *N+1*-component vectors belong to the moment space whose geometry is actually complex. Since it is difficult to figure out whether $(m_0,\ldots,m_N)^t$ belongs to the moment space, we consider from [4] derived quantities from the actual moment set. They are called canonical moments. We note them p_k. In order to define them we need to define the normalized moments, $c_k = m_k/m_0$. If $\boldsymbol{c}_{k-1} = (c_1, \ldots, c_{k-1})^t$ is in the interior of M_{k-1}, the set of all probability measures on [0,1] whose moments of order up to *k-1* are $\boldsymbol{c}_{k-1}$, $P(\boldsymbol{c}_{k-1})$, is infinite. Moreover, there exist two recursively defined boundaries, $c_{k-1}^{+} = \max_{\mu\in P(\boldsymbol{c}_{k-1})} c_{k-1}(\mu)$ and $c_{k-1}^{-} = \min_{\mu\in P(\boldsymbol{c}_{k-1})} c_{k-1}(\mu)$ with $c^{-}_{k-1} < c^{+}_{k-1}$, defining the admissible interval so that the vector of normalized moments $\boldsymbol{c}_k = (c_1,\ldots,c_k)^t$ belongs to the moment space M_k.

The canonical moment sequence $(p_k)_{k\le N}$ of this vector of moment can then be defined by $p_k = \dfrac{c_k - c^{-}_k}{c^{+}_k - c^{-}_k}$. According to their geometrical definition, each canonical moment lies in the interval [0,1], irrespective of the value of the other canonical moments. Besides, the canonical moments remain invariant under linear transformation of the distribution, i.e $\forall k \ge 1, p_k(f) = p_k(f_{S\min,S\max})$, where $f_{S\min,S\max}$ denotes the distribution induced by the linear transformation $S = S_{\min} + (S_{\max} - S_{\min})x$ of [0,1] onto $[S_{\min}, S_{\max}]$. That is another reason why we work on the size interval [0,1] without loss of generality. In the context of system (5), because we can prove that the canonical moments are transported quantities, i.e they satisfy $\partial_t p_k + \partial_x p_k \boldsymbol{u} = 0$. Therefore, they verify a maximum principle, and according to what precedes, provide a means to preserve the moment space.

The second difficulty lies in the fact that system (5) is weakly hyperbolic. When combining the first and the last equation, the velocity turns out to verify a transport equation $\partial_t \boldsymbol{u} + \boldsymbol{u}\partial_x \boldsymbol{u} = 0$ called the Burgers equation. It is typical of the pressureless gas structure [1], where velocity verifies a maximum principle. In this kind of model, when two droplets with different velocities meet, there can be shocks in velocity corresponding to the crossing of droplets trajectories which leads to mass concentration. This kind of singularity is called δ-shock. Meanwhile δ-shocks, a characteristic of the pressureless gas structure is the emergence of vacuum states.

Thus a numerical algorithm has to both preserve the moment space and maximum principles on the transported quantities which are satisfied by the original system of conservation equations.

Kinetic scheme and numerical algorithm for the advection of size moments

Because of the conservative form of system (5), the finite-volume method is a natural candidate for its discretization [1,2,3]. The underlying kinetic equation (3) with the corresponding closure for *f* is used for the derivation of a numerical flux formula that ensures the robustness of the corresponding scheme. In this context, it is called a kinetic scheme. Details of this scheme can be found in [1,2,3]. For a first order scheme, under the CFL condition, as piecewise constant data are used for the reconstruction, all the properties of system (5) are preserved: non negativeness of density, maximum principles on canonical moments (so that the moments stay in the moment space) and velocity.

However, we focus on applications where the description of the droplet cloud must be as precise as possible, which is the reason why we aim at designing a second order scheme. It is now essential to reconstruct the canonical moments, so that the scheme is conservative and satisfies maximum principles on them. Since there is no recursive dependence of the bounds for the canonical moments, an independent reconstruction of these quantities does not bring any problem. However, in order to strictly preserve the moment space, fluxes have to be computed precisely such as in kinetic schemes from these reconstructions using computer algebra using Maple (Maplesoft, a division of Waterloo Maple, Inc 2007). Let us insist on the fact that considering kinetic finite volume schemes and expressing the flux in terms of canonical moments enables to fully preserve the moment space.

Validation 1D results for the purely advection problem

We present a simple validation result where we use the aforementioned algorithm for a polydisperse droplet cloud in one dimension. The droplet cloud size distribution and initial velocity field are given by the following expressions:

$$f(x,S)=\begin{cases}4(0.5-x)\sin(\pi x)+(1-(4(0.5-x)^2)\exp(-S), & x\le 0.5\\ 0, & x>0.5\end{cases} \qquad v(x)=\begin{cases}0.5, & x\le 0.25\\ 1, & x>0.25\end{cases}$$

We set periodic boundary conditions on the space interval [0,1]. The analytical solution is the simple translation of the two parts of the density profile corresponding to each value of the velocity. The CFL number is 1, the number of cells is 400. Figure (1) displays the four analytical size moments, and the size moments given by the calculation at the time *t*=0.7 on the left, and at the time *t*=1.2 on the right. We can notice first that the moment space is preserved, and the numerical solution perfectly matches the analytical one. The initial distribution breaks into 2 parts. Vacuum is created at the initial velocity discontinuity. At *t*=1.2, the fastest portion catches up the slower one. As we consider prevents the particles from accumulating. However, it must be kept in mind that we do not take collision into account, and the real physical solution would result in a crossing of the clouds. Simulating jet crossing is an issue in Eulerian models and methods and has been recently resolved in the literature. We refer to [2] and references therein for details on this matter. Let us underline that our scheme can easily be extended to such cases and it is the material of a forthcoming paper. Thus we have validated our numerical approach in a simple case.

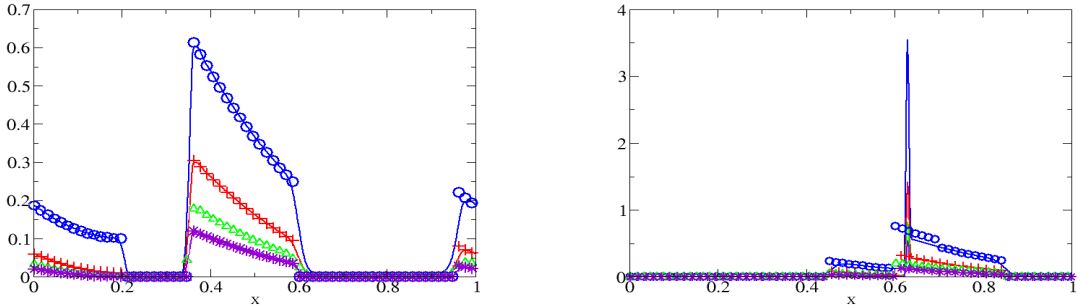

Figure 1: size moments at times *t*=0.7 (left) and *t*=1.2 (right). The markers represent the analytical solutions, and the curves represent the numerical solution : 0^{th} order moment (o), 1^{st} order moment (+), 2^{nd} order moment (Δ), 3^{rd} order moment (*)

Evaporation model

The advection model is now coupled with the evaporation model exposed in [9]. We recall here its main features. We consider only evaporation with d^2 law and take *R* to be -1 with standard non-dimensionalization (the typical time scale is the evaporation time based on the maximal droplet surface); the underlying kinetic equation then reads:

$$\partial_t f-\partial_S f=0 \qquad (5)$$

We use the same method as before, take the size moments on the [0,1] size interval of successive order up to 3 and derive the system of ordinary differential equations describing the evolution of the moments through evaporation:

$$\begin{aligned}\partial_t m_0 &= -f(t,0)\\ \partial_t m_1 &= -m_0\\ \partial_t m_2 &= -2m_1\\ \partial_t m_3 &= -3m_2\end{aligned} \qquad (6)$$

System (6) has to be closed, since the term $f(t,0)$, representing the disappearing flux of droplets at time *t*, is a pointwise value of the NDF which has to be related to values of moments in order to provide a closed system. This is a modeling as well as a numerical issue. Indeed once a value of f which makes system (6) stable (i.e staying in the moment space) has been determined, the numerical scheme has to preserve this stability. Finding these values amounts to solve the finite Hausdorff moment problem [4] for the set of moments $(m_0,...,m_n)^t$ in M_N .This is done using an Entropy Maximization [7]. However, when it comes to the numerical scheme, one has to evaluate the precise time evolution of this flux and we have proved in [7] that the kinetic schemes provide a dedicated tools which

relies on an integral formulation making use of the underlying kinetic equation. Using both ingredients, Entropy Maximization and a precise evaluation of the time evolution of the flux based on kinetic schemes allows to guarantee the preservation of the moment space and to solve an old issue in the literature.

Coupling transport in physical space and evaporation

As mentioned in the beginning, we use a splitting algorithm to separate the transport in physical space through convection and the transport in size phase space through evaporation. In order to keep the 2nd order property of both algorithms (for evaporation and transport), we use a Strang based splitting algorithm [2,3]. The interest is to preserve the properties of the schemes that we use for different contributions and it is computationally optimal and yields high parallelization capabilities. We focus now on results obtained with the model combining transport and evaporation. The initial conditions are the same as previously.. We then focus on the evaporation and transport of size moment at time 0.7. We compare the computed moments represented by solid lines in Fig.(2)-right to the analytical solutions represented by circles. This figure is to be compared with the left part of Fig.(1), with a lower scale here due to evaporation. We can see that the agreement is very good, which is an expected result since we use a high order method to describe polydispersity

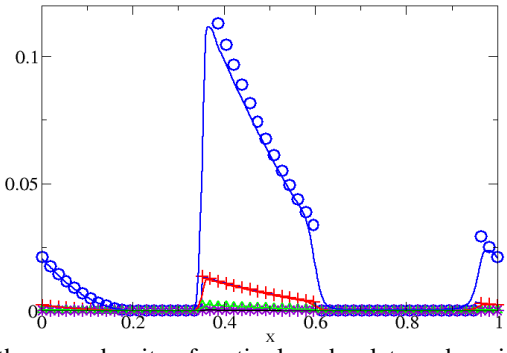

Figure 2: Left: Evolution of the mass density of motionless droplets undergoing evaporation: the solid curve represents the numerical solution, and the dashed curve represents the analytical solution. Right: Results at time *t=0.7* with evaporation and transport. The legend is the same as for Fig.(1)

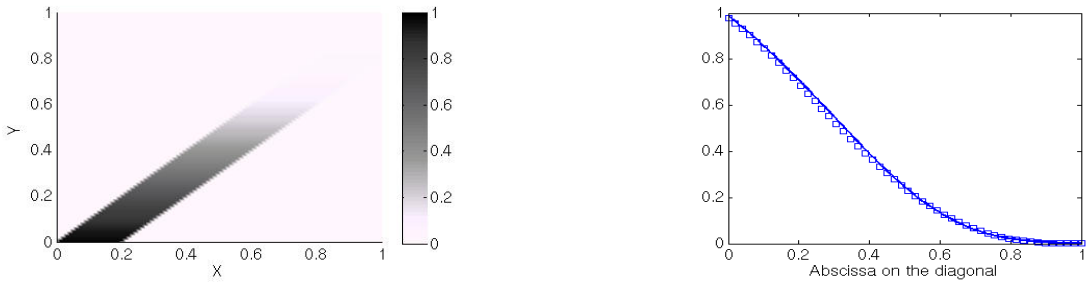

Figure 3: Left: Number density of the evaporative jet in two dimensions. Right: Comparison of the number density of the numerical (solid) and the corresponding analytical solution (circles) on the principal diagonal.

The second case deals with the injection of a jet in a 2*D* configuration. The spray is injected at the bottom left corner and goes to the upper right corner, with a velocity equals to 1 in the upper and right direction. The injected droplet number is 1, and Fig.(3)-left displays the evolution of this quantity. The CFL number is 1 and we use a 100×100 grid. Figure (3)-right compares the evolution of the number density along the principal diagonal between the numerical solution and the analytical solution. This test case displays the ability of the model and scheme to evaporate and transport a spray in two dimensions. As for the operator splitting, we use a dimensional splitting based on a Strang algorithm for the two dimensional solver.

Conclusion and perspective

In this article, we provide a comprehensive model accounting for evaporation and transport of a disperse droplet cloud. The main interest is that we have been able to devise an advection scheme which preserves moment interrelationships without using an extra algorithm to satisfy moment set validity concern. It is possible now to preserve the moment space and to minimize numerical diffusion, which seemed to be at odds in [10].

We provided in this article numerical tools whose final aim is to be implemented in a bi-fluid code, IFP-C3D [14]. This code simulates injection of fuel at high pressure and velocity into a gaseous cell, to access the spread of the fuel into the combustion chamber of car engines just before ignition. Nevertheless, the predictions of the liquid dynamics face an important limitation because the description of liquid polydispersity is not accurate, as its size distribution is just accessed through its volume fraction and interface density. Our aim is to implement the tools we displayed in this article in order to overcome the latter limitation and to do a step forward toward realistic predictions of the dynamics of two phase flow in internal combustion engines.

Nomenclature

- t: time
- $\boldsymbol{x}$: space
- S: surface of the particle
- $\boldsymbol{v}$: variable of the velocity phase space
- $f(t,\boldsymbol{x},S,\boldsymbol{v})$: size and velocity number density function
- $\boldsymbol{c}_n$: normalized moment vector of order n
- $n(t,\boldsymbol{x},S)$: size number density function
- M_n : moment space of order n
- m_n : size moment of order n
- c_n : normalized size moment of order n

References

[1] Bouchut F., Jin S, Li X., “Numerical approximations of pressureless and isothermal gas dynamics.”, *SIAM J. Num Anal, 41:135-158* (2003)

[2] de Chaisemartin S., Fréret L., Kah D., Laurent F., Fox R.O., Reveillon J. and Massot M., “Turbulent combustion of polydisperse evaporating sprays with droplet crossing: Eulerian modeling and validation in the infinite Knudsen limit”, *Proceeding of the Summer Program 2008: 265-276*, Center for Turbulence Research, Stanford University, to appear in a Special Issue of the *C. R. Acad. Sci. Paris* (2009)

[3] de Chaisemartin S., "Eulerian models and numerical simulation of turbulent dispersion of evaporating sprays*", Ph.D. Thesis of Ecole Centrale Paris* (2009)

[4] Dette H., Studden W.J., “The theory of canonical moments with applications in statistics, probability, and analysis.” Wiley Series in Probability and Statistics: Applied Probability and Statistics. J. Wiley & Sons Inc (1997)

[5] Greenberg J., Silverman I., Tambour Y., "On the origin of spray sectional conservation equations". *Combustion and Flame,* 93:90-96 (1993)

[6] Laurent F., Massot M., “Multi-Fluid modeling of laminar poly-dispersed spray flames: origin, assumptions and comparisons of the sectional and sampling methods”. *Combustion Theory and Modeling,* 5:537-572 (2001)

[7] Massot M., Laurent F., Kah D., De Chaisemartin S., “A robust moment method moment method for evaluating the disappearance rate of evaporating sprays.” *To appear in SIAM Journal of Applied Mathematics, available in HAL* (2009): http://hal.archives-ouvertes.fr/hal-00332423/fr/

[8] McGraw R., “Numerical advection of correlated tracers: Preserving particle size/composition moment sequences during transport of aerosol mixtures*.” Journal of Physics: Conference Series, 78* (2007)

[9] Wright D.L., “Numerical advection of moments of the particle size distribution in eulerian models.” Journal of Aerosol Science, pages 352-369 (2007)

[10] Zolver M., Klar D., Bohbot J. Laget O., Torres A., "reactive CFD in engines with a new unstructured parallel solver". *Oil and Gas Science and Technology*, 58:33-46 (2003)