



HAL
open science

Simulation of polydisperse oscillating droplets through high order numerical methods for geometric moment equations

Katia Ait-Ameur, Arthur Loison, Teddy Pichard, Marc Massot

► **To cite this version:**

Katia Ait-Ameur, Arthur Loison, Teddy Pichard, Marc Massot. Simulation of polydisperse oscillating droplets through high order numerical methods for geometric moment equations. The 11th International Conference on Multiphase Flow - ICMF 2023, Apr 2023, Kobe, Japan. hal-04934500

HAL Id: hal-04934500

<https://hal.science/hal-04934500v1>

Submitted on 7 Feb 2025

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Distributed under a Creative Commons Attribution 4.0 International License

Simulation of polydisperse oscillating droplets through high order numerical methods for geometric moment equations

Ait-Ameur Katia, Loison Arthur, Pichard Teddy and Massot Marc

Ecole Polytechnique, CMAP, Institut Polytechnique de Paris

Route de Saclay, Palaiseau, 91128, France

katia.ait-ameur@polytechnique.edu

Keywords: Two phase flow, polydisperse spray, moment method, kinetic finite volume scheme

Abstract

Liquid injection modeling and simulation face new challenges related to the need for predictive simulations in many fields such as combustion, chemical engineering, rocket booster propulsion and atmospheric studies. 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 polydisperse sprays with coupling capabilities to the separated phases zone is proposed in (Essadki & al 2019; Loison & al 2023) and, in the present contribution, we design specific numerical methods. The key ingredient in (Loison & al 2023) is a good choice of variables, which can describe both the polydisperse character of a spray as well as the geometrical dynamics of non spherical droplets. The resulting system of equations is hyperbolic but has a more complex structure; realizability conditions are satisfied at the continuous level, which imply a precise framework for numerical methods. To achieve the goals of accuracy, robustness and realizability, the kinetic finite volume schemes (Bouchut & al 2003) and Discontinuous Galerkin methods are promising numerical approaches (Cockburn & Shu 1998). We focus here on a two-phase simulation of a polydisperse spray with oscillating droplets and assess the ability of the model and of the related numerical methods to capture the physics of such flows.

Introduction

There is a need in many fields to model and simulate liquid injection from the moment it is injected until it becomes a cloud of polydisperse droplets. Models relying on a DNS framework can capture the whole jet dynamics for a limited range of Weber and Reynolds numbers. But both the computational resources required as well as the modeling and physics of topology changes at small scales, make it unaffordable in terms of the range of scales to be resolved for realistic conditions of industrial interest. Reduced order models are then a powerful alternative as it allows computations to be done at a reasonable cost.

Two families of reduced models can be found. The first one, the class of two-fluid models, provides an Eulerian description of the dense liquid region close to the injector, referred to as separate phase flow. It provides some level of description of the interface geometry depending on the modeling assumptions.

The second modeling family relies on a statistical description of the particles/droplets far from injection when the atomization process has been fully completed. The particle properties are monitored by a number density function (NDF) that is solution of a kinetic equation. Since the direct resolution of the kinetic equation is often intractable due to the large number of independent variables, Eulerian moment methods can be a promising alternative for an approximate

resolution. In this approach, we consider the moments of the NDF over a phase space that describes the dynamics of the droplets. The choice of the moments set and of the closure hypotheses depend on the level of the description needed to capture some features of the spray like the polydispersion or the deformations of the droplets that can be non spherical. The disperse phase is obtained from the atomization of the liquid jet in the separated phases zone, where the gas-liquid interface geometry has an important influence on the atomization process. It is then important to find a set of the moments that can be extended and related to some intrinsic variables in the separated phases. In (Loison & al 2023), the authors propose a high order moment model for polydisperse spray that takes into account the oscillatory characteristics of the droplets. The choice of the moments set is motivated by geometric variables of the interface topology such as the interfacial area density. These geometric variables can also enrich the subscale modelling of the interface within a two-fluid model describing the separated phases flow.

In this contribution, we are interested in developing numerical methods for the approximation of the moments model based on geometric variables (Loison & al 2023). There exists a stumbling block for the usual approaches using high order moment method resolved with at least second-order numerical methods. The transport algorithm does not systematically preserve the moment space, which means that slope reconstruction of moments by piecewise polynomials

are likely to create vectors whose components fail to be the moments of a distribution. One way to resolve this is to impose a posteriori to the moment vector to stay inside the realizable moment space.

Moments model and realizable numerical methods

The spray of droplets is described by a NDF $f(t, x, v, S_0, \xi, \dot{\xi})$. It provides the number of droplets whose position, velocity and oscillatory characteristics lie in a small volume $dS_0 d\xi d\dot{\xi} dx dv$. We assume that the velocity v of the droplets is the same as the surrounding gas u :

$$f(t, x, v, S_0, \xi, \dot{\xi}) = n(t, x, S_0, \xi, \dot{\xi})\delta(v - u(t, x)). \quad (1)$$

The NDF is solution of a Williams-Boltzmann equation modeling the transport of droplets carried by a gaseous flow.

$$\partial_t n + \nabla_x \cdot (nu) + \partial_\xi(\Xi(S_0, \xi, \dot{\xi})n) + \partial_{\dot{\xi}}(\ddot{\Xi}(S_0, \xi, \dot{\xi})n) = 0 \quad (2)$$

In general, this equation is too expensive to solve by a simple discretization of the phase space $(S_0, \xi, \dot{\xi})$. Reduced-order models are proposed in (Essadki & al 2019; Loison & al 2023) based on specific geometric moments of n . The choice of the moment set is critical for the existence of a NDF. For the monovariate problem in size $n(t, x, S_0)$, the choice of the moments is based on a set of geometrical variables describing the interface topology of the droplet population.

- the volume fraction variables $\alpha = \frac{1}{6\sqrt{\pi}}m_{3/2}$;
- the interfacial area density $\Sigma = m_1$;
- the Gauss $\hat{G} = 4\pi m_0$ and mean curvatures $\hat{H} = \sqrt{\pi}m_{1/2}$.

where the moments $m_{k/2}$ of order $k/2$ are defined by:

$$m_{k/2}(t, x) = \int_0^1 S^{k/2} n(t, x, S) dS. \quad (3)$$

For the solution of moments models, accurate and robust numerical methods are mandatory in order to handle the numerical difficulties. The monokinetic assumption (1) yields to weakly hyperbolic systems, which present some difficulties like void regions and singularities. Furthermore, moment models require that the numerical scheme satisfies the realizability condition (every set of moments has to be associated with a NDF) in each cell. To fulfill these conditions, one can use kinetic schemes (Bouchut & al 2003) by using the exact solution in time of the underlying kinetic description (2). On the other hand, in the literature, several high order numerical schemes can be found for the resolution of hyperbolic system of equations. In order to meet all these properties, i.e. realizability preservation and high order of accuracy, a class of Runge-Kutta Discontinuous Galerkin scheme is used (Cockburn & Shu 1998).

Results and Discussion

In this contribution, we provide a new method for the transport in physical space of droplet distribution using Runge

Kutta Discontinuous Galerkin methods. We propose a new approach as well as an algorithm which is arbitrarily high order in space and time with low numerical diffusion (Ait-Ameur & al 2023). This allows to accurately describe the advection process and naturally guarantees that the vector always belongs to the moment space if the initial solution itself belongs to the moment space. These schemes stay robust even when facing the severe singularities created by the models, especially δ -shocks and vacuum zones.

Conclusion

In order to obtain accurate and robust results, the systems of equations resulting from (Essadki & al 2019; Loison & al 2023) should be solved with realizability-preserving high order methods. The kinetic finite volume schemes and the RKDG methods were shown to be competitive for the description of the spray dynamics. These schemes can accurately reproduce the high preferential concentration that characterizes the dynamics of low inertia particles as well as the right segregation level. The accurate description of these quantities is essential in the domain of sprays since they affect the local mixture fraction and the evaporation rate.

The extension of this numerical strategy to the multivariate case $n(t, x, S_0, \xi, \dot{\xi})$ is an on going work. It will allow us to simulate a cloud of non spherical droplets by taking into account the geometrical dynamics described by the phase variables $(\xi, \dot{\xi})$.

Acknowledgments

This work was supported by a grant from Region Ile-de-France DIM MATHINNOV and the DGA project MMEED.

References

- K. Ait-Ameur, M. Essadki, S. Kokh, M. Massot and T. Pichard. Limitation strategies for high-order discontinuous Galerkin schemes applied to Eulerian models of polydisperse sprays. In preparation. (2023).
- F. Bouchut, S. Jin, and X. Li. Numerical approximations of pressureless and isothermal gas dynamics, *SIAM J. Num. Anal.*, 41, pp. 135-158. (2003)
- B. Cockburn and C.-W. Shu. The Runge-Kutta Discontinuous Galerkin method for conservation laws V, *Journal of Computational Physics*, 141, pp. 199-224. (1998)
- M. Essadki, F. Drui, S. de Chaisemartin, A. Larat, T. Ménard and M. Massot. Statistical modeling of the gas-liquid interface using geometrical variables: toward a unified description of the disperse and separated phase flows. *Int. J. Multiphase Flow*, 120, 204-216. (2019).
- A. Loison, S. Kokh, M. Massot and T. Pichard. Two-phase flow reduced-order model : a two-scale model of polydisperse oscillating droplets. In preparation. (2023).