

Eulerian models for the description of polydisperse sprays : from fundamental issues to industrial applications and HPC

M. Massot

Laboratoire EM2C, UPR CNRS 288 – Ecole Centrale Paris –
Fédération de Mathématiques de l’Ecole Centrale Paris - FR CNRS 3487
marc.massot@ecp.fr

The modeling and simulation of multiphase reacting flows covers a large spectrum of applications ranging from combustion in automobile and aeronautical engines to atmospheric pollution as well as biomedical engineering. In the framework of this seminar, we will mainly focus on a disperse liquid phase carried by a gaseous flow field which can be either laminar or turbulent; however, this spray can be polydisperse, that is constituted of droplets with a large size spectrum. Thus, such flows involve a large range of temporal and spatial scales which have to be resolved in order to capture the dynamics of the phenomena and provide reliable and eventually predictive simulation tools. Even if the power of the computer resources regularly increases, such very stiff problems can lead to serious numerical difficulties and prevent efficient multi-dimensional simulations.

The purpose of this seminar is to introduce to the Eulerian modeling of polydisperse evaporating spray for various applications, that is the disperse liquid phase carried by a gaseous flow field is modeled by ‘fluid’ conservation equations. Such an approach is very competitive for real applications since it has strong ability for optimization on parallel architectures and leads to an easy coupling with the gaseous flow field resolution. We will show that all the necessary steps in order to develop a new generation of computational code have to be designed at the same time with a high level of coherence: mathematical modeling through Eulerian moment methods, development of new dedicated stable and accurate numerical methods, implementation of optimized algorithms as well as verification and validations of both model and methods using other codes and experimental measurements.

We will introduce both a new class of models and their mathematical analysis for the direct numerical simulation of spray dynamics [1, 2, 3, 4, 5, 6, 7] even in the presence of coalescence and break-up [8], as well as a set of dedicated numerical methods [1, 9, 10, 2, 11, 8, 12] and prove that such an approach has the ability, once validated [13], to lead to high performance computing on parallel architectures [14]. We will finally present a synthesis of recent contributions, which aim at: 1- on the one side transferring the proposed models into identified codes for industrial applications in the fields of solid propulsion, aeronautical and automotive engines [15, 12, 16], 2- on the other side extending the previous work to turbulent flows, where some scales can not be resolved and have to be modeled, and where some dedicated numerical methods have to be designed [17, 18, 19].

References

- [1] M. Massot, F. Laurent, S. de Chaisemartin, L. Fréret, and D. Kah. Eulerian multi-fluid models: modeling and numerical methods. In *Modelling and Computation of Nanoparticles in Fluid Flows*, Lectures Notes of the von Karman Institute, pages 1–86. NATO RTO-EN-AVT-169, 2009. <https://www.cso.nato.int/pubs/rdp.asp?RDP=RTO-EN-AVT-169>.
- [2] 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 Paris, France, 2010. in English, <http://tel.archives-ouvertes.fr/tel-00618786/>.
- [3] 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. App. Math.*, 70(8):3203–3234, 2010.
- [4] D. Kah, F. Laurent, M. Massot, and S. Jay. A high order moment method simulating evaporation and transport of a polydisperse liquid spray. *J. Comp. Phys.*, 231:394–422, 2012.

- [5] D. Kah, F. Laurent, L. Fréret, S. de Chaisemartin, R. O. Fox, J. Reveillon, and M. Massot. Eulerian quadrature-based moment models for dilute polydisperse evaporating sprays. *Flow, Turbulence and Combustion*, 85(3-4):649–676, 2010.
- [6] C. Chalons, D. Kah, and M. Massot. Beyond pressureless gas dynamics: quadrature-based velocity moment models. *Com. Math. Sci.*, 10:1241–1272, 2012.
- [7] A. Vié, F. Laurent, and M. Massot. Size-velocity correlations in hybrid high order moment/multi-fluid methods for polydisperse evaporating sprays: modeling and numerical issues. *Journal of Computational Physics*, 237:277–310, 2013.
- [8] F. Doisneau, F. Laurent, A. Murrone, J. Dupays, and M. Massot. Eulerian multi-fluid models for the simulation of dynamics and coalescence of particles in solid propellant combustion. *J. Comput. Phys.*, 234:230–262, 2013.
- [9] S. de Chaisemartin. *Eulerian models and numerical simulations of turbulent dispersion of polydisperse evaporating sprays*. PhD thesis, Ecole Centrale Paris, France, 2009. in English, <http://tel.archives-ouvertes.fr/tel-00443982/>.
- [10] S. de Chaisemartin, L. Fréret, D. Kah, F. Laurent, R.O. Fox, J. Reveillon, and M. Massot. Eulerian models for turbulent spray combustion with polydispersity and droplet crossing. *Comptes Rendus Mécanique*, 337:438–448, 2009. Special Issue 'Combustion for Aerospace Propulsion'.
- [11] F. Doisneau. *Eulerian modeling and simulation of polydisperse moderately dense coalescing spray flows with nanometric-to-inertial droplets: application to Solid Rocket Motors*. PhD thesis, Ecole Centrale Paris, 2013.
- [12] F. Doisneau, A. Sibra, J. Dupays, A. Murrone, F. Laurent, and M. Massot. An efficient and accurate numerical strategy for two-way coupling in unsteady polydisperse moderately dense sprays: application to Solid Rocket Motor instabilities. *Journal of Propulsion and Power*, 30:727–748, 2014.
- [13] L. Fréret, C. Lacour, S. de Chaisemartin, S. Ducruix, D. Durox, F. Laurent, and M. Massot. Pulsated free jets with polydisperse spray injection: Experiments and numerical simulations. *Proceedings of the Combustion Institute*, 32(2):2215–2222, 2009.
- [14] L. Fréret, O. Thomine, J. Reveillon, S. de Chaisemartin, F. Laurent, and M. Massot. On the role of preferential segregation in flame dynamics in polydisperse evaporating sprays. In *Proceedings of the Summer Program 2010, Center for Turbulence Research, Stanford University*, pages 383–392, 2010.
- [15] A. Vié, S. Jay, B. Cuenot, and M. Massot. Accounting for polydispersion in the eulerian large eddy simulation of an aeronautical-type configuration. *Flow, Turbulence and Combustion*, 90:545–581, 2013.
- [16] D. Kah, O. Emre, Q.H. 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*, pages 1–42, 2014. To appear, <http://hal.archives-ouvertes.fr/hal-00941796>.
- [17] A. Vié, E. Masi, O. Simonin, and M. Massot. On the direct numerical simulation of moderate-stokes-number turbulent particulate flows using Algebraic-Closure-Based and Kinetic-Based Moment Methods. In *Proceedings of the Summer Program 2012, Center for Turbulence Research, Stanford University*, pages 355–364, 2012.
- [18] A. Vié, F. Doisneau, and M. Massot. On the Anisotropic Gaussian closure for the prediction of inertial-particle laden flows. *Communication in Computational Physics*, pages 1–48, 2014. in Press, <http://hal.archives-ouvertes.fr/hal-00912319>.
- [19] F. Doisneau, O. Thomine, F. Laurent, A. Vié, J. Dupays, and M. Massot. Eulerian modeling and simulation of small scale trajectory crossing and coalescence for moderate-Stokes-number spray flows. In *Proceedings of the Summer Program 2012, Center for Turbulence Research, Stanford University*, pages 365–374, 2012.