Available online at www.sciencedirect.com
ScienceDirect
C. R. Acad. Sci. Paris, Ser. I 347 (2009) 691–696
COMPTES RENDUS MATHEMATIQUE

Mathematical Problems in Mechanics

A moment method for polydisperse sprays

Lukas Schneider [a,*], Nechtan Le Lostec [b], Philippe Villedieu [b], Amsini Sadiki [a]

[a] *TU Darmstadt, EKT, Petersenstrasse 30, 64287 Darmstadt, Germany*
[b] *ONERA, 2, avenue Edouard-Belin, 31055 Toulouse, France*

Received 28 August 2008; accepted after revision 24 March 2009

Available online 10 April 2009

Presented by Olivier Pironneau

Abstract

This Note outlines a new moment method to solve the kinetic spray equation, which is the basic mathematical model used to predict the behaviour of polydisperse sprays. The method was successfully applied to the test-cases of spray-wall impingement and crossing of two spray jets that were affected by the Stokes drag force. Lagrangian computations of the same test-cases were used as reference solutions. ***To cite this article: L. Schneider et al., C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Résumé

Une méthode de moments pour la modélisation des sprays polydisperses. Dans cette Note, nous proposons une nouvelle méthode de moments pour la modélisation des sprays, permettant de traiter des situations de fort déséquilibre, dans lesquelles la fonction de distribution caractérisant le brouillard est localement multimodale vis à vis de la taille ou de la vitesse des gouttes. Cette méthode a été appliquée avec succès aux cas de l'éclaboussement d'un spray sur une paroi et du croisement de deux jets de granulométries différentes. ***Pour citer cet article : L. Schneider et al., C. R. Acad. Sci. Paris, Ser. I 347 (2009).***

Version française abrégée

Les écoulements gaz-gouttelettes – ou *sprays* – interviennent dans de nombreuses applications (moteurs à combustion, systèmes de refroidissement par sprays, débitmètres diphasiques pour n'en citer que quelques unes) si bien que le développement de méthodes de simulation numérique précises et efficaces constitue un enjeu important pour l'industrie. Actuellement, deux approches sont couramment utilisées : l'approche dite « lagrangienne » [6] qui consiste à résoudre, à l'aide d'une méthode particulaire stochastique, l'équation cinétique (1) modélisant l'évolution du spray, et l'approche dite « eulérienne » [4,5,3] qui repose sur la résolution, à l'aide d'une méthode de volumes finis, d'un système de lois de conservation portant sur certains moments privilégiés de la fonction de distribution décrivant la phase disperse (notée f dans la suite de cette Note). Sur le plan numérique, l'approche eulérienne est plus précise et d'un

* Corresponding author.
E-mail addresses: schneider@ekt.tu-darmstadt.de (L. Schneider), Nechtan.Le_Lostec@onecert.fr (N. Le Lostec), Philippe.Villedieu@onecert.fr (P. Villedieu), sadiki@ekt.tu-darmstadt.de (A. Sadiki).

1631-073X/$ – see front matter
doi:10.1016/j.crma.2009.03.023

coût plus faible que l'approche lagrangienne, en particulier pour la simulation des écoulements instationnaires. Par contre, elle requiert des hypothèses sur la forme de la fonction f vis à vis des variables de taille et de vitesse (rayon et vitesse des gouttes) afin de fermer le système des moments à un certain ordre (un ou deux pour les modèles proposés dans la littérature). Ces hypothèses ne sont pas nécessairement vérifiées dans les applications traitées, en particulier dans les situations de fort déséquilibre telles que l'éclaboussement d'un spray sur une paroi ou le croisement de deux jets de gouttes, et les résultats obtenus peuvent alors être trés éloignés de la solution physique (correspondant à la solution de l'équation cinétique).

Dans cette Note, nous proposons une nouvelle méthode de moments basée sur la relation (4) pour l'approximation de la fonction de distribution. Il est important de souligner que (4) constitue – au moins formellement – une formule générale d'approximation et ne doit donc pas être interprétée comme une simple relation de fermerture, même si, à I et N fixés, elle peut, a posteriori, être vue comme telle. Les degrés de liberté, b_k, a_k^i, U_k^i, étant au nombre de $(2I+1)N$, il est nécessaire, dans le cas général, de résoudre un système de lois de conservation pour un ensemble de $(2I+1)N$ moments définis par la relation $(3)_2$. La méthode décrite ici peut être vue comme une généralisation de la méthode sectionnelle [4,5] – ou plus exactement de sa variante à deux degrés de liberté par section proposée par Dufour et Villedieu [2] – et de la méthode de quadrature récemment introduite dans [1], puisqu'en effet (4) redonne la méthode de [2] dans le cas $I=1$ et, à quelques nuances près, celle de [1] dans le cas $N=1$.

Pour des raisons de coût évidentes, il est essentiel de vérifier qu'il est possible d'obtenir une précision suffisante en se limitant à de faibles valeurs pour I et N. Les résultats numériques présentés dans cette Note correspondent aux choix $N=5$, 10, 20 et $I=2$. Afin de valider la méthode proposée, dans les situations où les méthodes eulériennes usuelles sont connues pour ne pas donner une solution satisfaisante, nous avons traité deux cas de calculs : le cas du croisement de deux jets dilués (sans collision) et celui de l'éclaboussement d'un spray sur une paroi (avec un modèle d'interaction simple). Nous avons comparé les résultats obtenus à ceux fournis par une méthode lagrangienne. Avec seulement 5 sections, on constate (cf. Figs. 1 et 2) que l'accord entre les deux approches est tout à fait satisfaisant. D'autres tests sont actuellement en cours, en une et deux dimensions d'espace, prenant également en compte les phénomènes d'évaporation. Les résultats de ces tests ainsi qu'une description détaillée de la méthode numérique utilisée feront l'objet d'une prochaine publication [7].

1. Introduction

In this work a new method for the prediction of spray phenomena is presented which can be regarded as an alternative to the classical Lagrangian and Eulerian procedures. It will be demonstrated that this method captures the polydisperse nature of sprays as well as the coexistence of two (or more) droplet velocities at one location.

The Lagrangian procedure (cf. [6]), also called particle stochastic method, solves the kinetic spray equation by solving the motion of a large number of numerical particles, so-called parcels, in phase space. For highly unsteady flows, this method requires a nearly unmanageable amount of parcels to deliver smooth statistics. In addition, the parallelisation technique of dividing the computational domain into equisized sub domains does not ensure the desired linear scaling of the computational time with the processors.

Describing the spray behaviour with an Eulerian method, i.e. solving balance equations for various densities of physical droplet quantities at each point of the domain, has the advantage, that irrespective of the amount of droplets in a region, the same number of equations always have to be solved. Consequently, the above problem of parallelisation does not arise and the unsteady character of the flow can be treated with higher order time and space discretisations. Nevertheless, the application of an Eulerian description has its limitations. By using a two fluid model, i.e. solving two superposed and coupled sets of Navier–Stokes-like equations to describe the droplet and gas behaviour (cf. [3]), the polydisperse character of the spray can only be captured in a very crude manner. One way to resolve this problem is the sectional method (cf. [4,5,2]), which is able to predict polydisperse effects of the droplets accurately. Still, it does not allow the dispersion of droplet velocities at one location which is necessary, for example, to capture the crossing of two dilute sprays. Recently, in [1] a quadrature-based moment method was proposed that overcomes this drawback by solving balance equations not only for the number, mass and momentum densities but also for higher order moments of the droplet number density function.

After introducing a kinetic model for polydisperse sprays in Section 2, the idea of Desjardins et al. [1] is followed and combined with the propositions of Dufour and Villedieu [2] in Section 3. This combination allows for the description of changes in the droplet size distribution and at the same time considers the droplet velocity dispersion at one

location. In Section 4 the new method is compared to a reference Lagrangian method, first in a one-dimensional setting of two crossing spray distributions that are decelerated by a Stokes drag force and secondly in a configuration where droplets are reflected on a wall but break and lose mass and momentum (hereafter called splashing). Conclusions are drawn in Section 5.

2. Mathematical model of polydisperse sprays

Similar to the description of molecules in the kinetic gas theory, Williams [8] proposed a general type of equation to model the behaviour of spray systems. Here, the reduced version

$$\frac{\partial f}{\partial t} + \frac{\partial (vf)}{\partial x} + \frac{\partial (\mathrm{F}f)}{\partial v} = 0 \tag{1}$$

of the general spray model is used which, for simplicity, does not include the thermodynamic and interaction behaviour of droplets. In Eq. (1), f is a function of time t, space x, droplet velocity v and a scalar that characterises the droplet size s (here, the droplet surface). It is physically interpreted as number of droplets per infinitesimal volume $[x, x+\mathrm{d}x] \times [v, v+\mathrm{d}v] \times [s, s+\mathrm{d}s]$ and is therefore called number density function. The forces on the droplets of the type $\mathrm{F} = (U_g(t,x) - v)/\tau_d(s,v)$, which excludes gravity, buoyancy and other, more subtle forces are considered. The above drag force model includes the velocity difference between a droplet and the gas, $(U_g - v)$, and the relaxation time of the droplets in the surrounding gas, τ_d. In the remainder of this Note the one-dimensional version of Eq. (1) is dealt with,

$$\frac{\partial f}{\partial t} + \frac{\partial (vf)}{\partial x} + \frac{\partial}{\partial v}\left(\frac{U_g - v}{St(s,v)} f\right) = 0, \tag{2}$$

in which all quantities are disposed of their units. For the definition of the Stokes number, $St = \tau_d/\tau_g$, the characteristic time scale for the gas flow, τ_g, is introduced.

3. Moment closure

The moment transform in s- and v phase-space is performed by using the set of moments (cf. [1,2])

$$\mathcal{V}_k := \left\{\mathrm{M}^{(k)}_{0,0}, \mathrm{M}^{(k)}_{3/2,0}, \mathrm{M}^{(k)}_{3/2,1}, \mathrm{M}^{(k)}_{3/2,2}, \mathrm{M}^{(k)}_{3/2,3}\right\}, \qquad \mathrm{M}^{(k)}_{K,L}(t,x) := \int_{s_k}^{s_{k+1}} s^K \int_{\mathbb{R}} v^L f(t,x,s,v)\,\mathrm{d}v\,\mathrm{d}s, \tag{3}$$

in each of the N fixed intervals $I_k = [s_k, s_{k+1}] \in [0,1]$, called sections. The balance equations for the above moments are derived by multiplying the reduced spray equation (2) with the appropriate powers of the phase-space variables and integrating the emerging equations over the whole velocity phase-space and each section I_k. This set of $5N$ moment equations is not closed, because in the equation for $\mathrm{M}^{(k)}_{3/2,3}$ the unspecified moment $\mathrm{M}^{(k)}_{3/2,4}$ arises. In addition, the integral

$$\int_{s_k}^{s_{k+1}} s^K \int_{\mathbb{R}} v^L \frac{\partial}{\partial v}\left(\frac{U_g - v}{St} f\right) \mathrm{d}v\,\mathrm{d}s$$

which is part of each of these equations cannot be evaluated unless the generality of f has been reduced. Here, U_g is given by some analytical or numerical solution of the gas flow and St is modelled by the Stokes law.

The moment equations are closed by assuming the number density function to have the form

$$\tilde{f}(t,x,s,v) = \sum_{k=1}^{N} \sum_{i=1}^{I} \mathbf{1}_{s_k \leqslant s \leqslant s_{k+1}} a^i_k(t,x) \exp\bigl(-b_k(t,x)s\bigr) \delta_{v - U^i_k(t,x)} \tag{4}$$

with $I = 2$. This closure allows the emerging moment equations to be solved with the available numerical methods and, more importantly, it does not contradict the velocity dispersion and the polydisperse nature of sprays (see Section 4). Furthermore, it is to remark that, as indicated in (4), any value of I is admissible to describe the velocity

dispersion at one location. If the number density function f is replaced with its approximation $\tilde{f}$ the following closed system of equations for the set of moments $\mathcal{V}_k$ is obtained,

$$\frac{\partial}{\partial t}\big(\mathrm{M}^{(k)}_{0,0}\big)+\frac{\partial}{\partial x}\big(\mathrm{M}^{(k)}_{0,1}\big)=0,\qquad \frac{\partial}{\partial t}\big(\mathrm{M}^{(k)}_{3/2,0}\big)+\frac{\partial}{\partial x}\big(\mathrm{M}^{(k)}_{3/2,1}\big)=0,\ldots,$$
$$\frac{\partial}{\partial t}\big(\mathrm{M}^{(k)}_{3/2,3}\big)+\frac{\partial}{\partial x}\big(\mathrm{M}^{(k)}_{3/2,4}\big)=3\int_{s_k}^{s_{k+1}} s^{3/2}\exp(-b_k s)\left[a_k^1\big(U_k^1\big)^2\frac{U_g-U_k^1}{St(U_k^1,s)}+a_k^2\big(U_k^2\big)^2\frac{U_g-U_k^2}{St(U_k^2,s)}\right]\mathrm{d}s. \tag{5}$$

In each section, $\tilde{f}$ is defined by five parameters that are linked to the moments in $(3)_1$. It is straight forward to compute the moments in set $\mathcal{V}_k$ from the set of parameters, $\mathcal{W}_k=[b_k,a_k^1,a_k^2,U_k^1,U_k^2]$, by simply inserting $\tilde{f}$ into the definitions $(3)_2$ of the moments. The inverse problem of uniquely determining the parameters $\mathcal{W}_k$ from the moments $\mathcal{V}_k$ is the subject of Theorem 3.1. It constitutes the main part of the numerical algorithm to solve the moment equations (5).

Theorem 3.1. *Let $\mathcal{V}_k$ be the set of moments defined in* (3) *such that*

$$\text{(i) } \mathrm{M}^{(k)}_{0,0}>0,\quad \text{(ii) } \mathrm{M}^{(k)}_{3/2,0}>0,\quad \text{(iii) } \mathrm{M}^{(k)}_{3/2,2}\geqslant\frac{(\mathrm{M}^{(k)}_{3/2,1})^2}{\mathrm{M}^{(k)}_{3/2,0}}\quad \textit{and}\quad \text{(iv) } \frac{\mathrm{M}^{(k)}_{3/2,0}}{\mathrm{M}^{(k)}_{0,0}}\in\big]s_k^{3/2},s_{k+1}^{3/2}\big[, \tag{6}$$

then, up to a permutation between subscripts 1 *and* 2*, there exists only one set $\mathcal{W}_k$ of parameters that solves the inverse problem. This solution is given by the inverse function*

$$b_k=g_k^{-1}\left(\frac{\mathrm{M}^{(k)}_{3/2,0}}{\mathrm{M}^{(k)}_{0,0}}\right)\quad \textit{with } g_k(b):=\begin{cases}\dfrac{2}{5}\dfrac{(s_{k+1}^{5/2}-s_k^{5/2})}{|I_k|}, & b=0,\\[2ex] \dfrac{\int_{s_k}^{s_{k+1}} s^{\frac{3}{2}}\exp(-b_k s)\,\mathrm{d}s}{\int_{s_k}^{s_{k+1}}\exp(-b_k s)\,\mathrm{d}s}, & b\neq 0,\end{cases} \tag{7}$$

and the relations

$$a_k^1=(1/2+x_k)\big(\bar{\mathrm{M}}^{(k)}_{3/2,0}\big),\qquad a_k^2=(1/2-x_k)\big(\bar{\mathrm{M}}^{(k)}_{3/2,0}\big),$$
$$U_k^1=U_k^p-\left(\frac{a_k^2}{a_k^1}\right)^{1/2}\sigma_k^p,\qquad U_k^2=U_k^p+\left(\frac{a_k^1}{a_k^2}\right)^{1/2}\sigma_k^p,\qquad x_k=\frac{q_k^p/2}{((q_k^p)^2+4(\sigma_k^p)^6)^{1/2}}. \tag{8}$$

The quantities $\bar{\mathrm{M}}^{(k)}_{3/2,0}$, U_k^p, σ_k^p and q_k^p are defined by

$$\bar{\mathrm{M}}^{(k)}_{3/2,0}=\frac{\mathrm{M}^{(k)}_{3/2,0}}{\int_{s_k}^{s_{k+1}} s^{\frac{3}{2}}\exp(-b_k s)\,\mathrm{d}s},\qquad U_k^p=\frac{\bar{\mathrm{M}}^{(k)}_{3/2,1}}{\bar{\mathrm{M}}^{(k)}_{3/2,0}},\qquad \sigma_k^p=\left(\frac{\bar{\mathrm{M}}^{(k)}_{3/2,0}\bar{\mathrm{M}}^{(k)}_{3/2,2}-(\bar{\mathrm{M}}^{(k)}_{3/2,1})^2}{(\bar{\mathrm{M}}^{(k)}_{3/2,0})^2}\right)^{1/2},$$
$$q_k^p=\frac{1}{\bar{\mathrm{M}}^{(k)}_{3/2,0}}\big(\bar{\mathrm{M}}^{(k)}_{3/2,3}-\bar{\mathrm{M}}^{(k)}_{3/2,0}\big(U_k^p\big)^3-3\big(\bar{\mathrm{M}}^{(k)}_{3/2,0}\big)\big(\sigma_k^p\big)^2U_k^p\big). \tag{9}$$

Eqs. (7) *to* (9) *constitute the mapping $\mathcal{V}_k\longrightarrow\mathcal{W}_k$.*

Sketch of the proof for Theorem 3.1. *It was proven in* [2] *that $g_k(b)$ is a strictly decreasing function on $\mathbb{R}$ with the properties:* $\lim_{b\to-\infty} g_k(b)=s_{k+1}^{3/2}$ *and* $\lim_{b\to+\infty} g_k(b)=s_k^{3/2}$*. Therefore, using* (iv) *in each section, g_k can be inverted and a unique solution b_k can be found from Eq.* (7)*. With the solution for b_k and* (i), (ii) *and* (iii) *we refer to* [1] *for the proof that, up to a permutation of $(a_q^1,\mathbf{U}_q^1)$ with $(a_q^2,\mathbf{U}_q^2)$, $\mathcal{W}_k$ is uniquely determined by the set $\bar{\mathcal{V}}_k=\{\bar{\mathrm{M}}^{(k)}_{0,0},\bar{\mathrm{M}}^{(k)}_{3/2,0},\bar{\mathrm{M}}^{(k)}_{3/2,1},\bar{\mathrm{M}}^{(k)}_{3/2,2},\bar{\mathrm{M}}^{(k)}_{3/2,3}\}$ of normalised moments.*

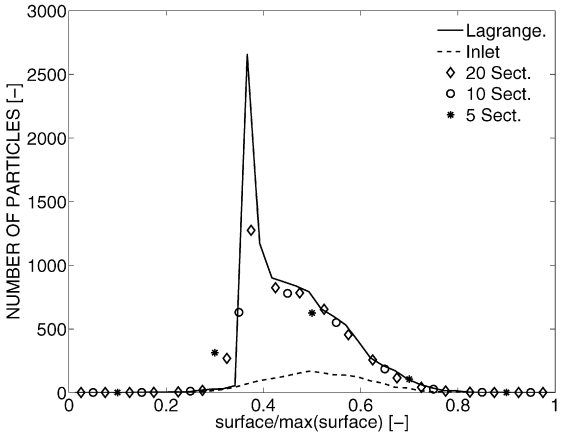

Fig. 1. Crossing of two jets and Stokes drag $St_{max} = 2.43$.

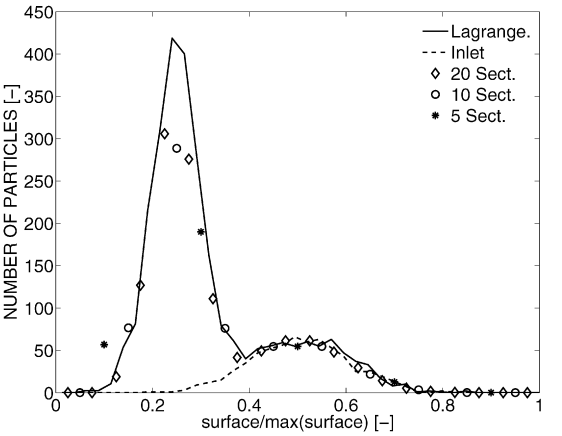

Fig. 2. Splashing with $\alpha = 0.9$, $\beta = 0.7$, $\gamma = 0.1$.

4. Test cases: drag and splashing

The method outlined above was applied to two test-cases that change the distribution of droplets in surface phase-space, first, through a size-dependent drag force, and second, through splashing. Both test-cases were organised in such a way that crossing of two different droplet distributions was included. Solutions to the same test-cases were also computed using a Lagrangian method. They are regarded as accurate reference solutions. The numerical algorithms for these tests will be explained in [7].

In the drag test-case two truncated Gaussian distributions of droplets in surface phase-space, with the same mean value, variance and initial velocity, are moving towards each other. Both distributions are affected by the Stokes drag that results from the velocity difference between the non-moving air and the water-droplets. The size and initial velocities of the droplets are chosen such that the two distributions cross each other. Fig. 1 depicts the number distribution of droplets for the various solutions versus the surface variable at the point 7/8*length of domain after 5.0 time units. It is observed that the strong concentration of mass due to the standstill of droplets (see sharp peak) can only be captured by using 20 sections, whereas the properties of moving droplets can be predicted by all solutions.

In the splashing test-case the same Gaussian distribution enters the domain from the left and is freely transported through it. At the right boundary the spray is reflected, but speed reduces by a factor of α, diameter by a factor of β and a fraction γ of its mass is lost. In Fig. 2 the number of droplets in each section, at point 3/4*length of domain is compared to the steady state, Lagrangian results. The high peak on the left side represents the splashed spray and is moving away from the wall, whereas the smaller peak on the right, agreeing with the inlet distribution (dashed line), is moving towards the wall. It is observed that splashing is well captured by calculations with 20 sections and that reduction of the number of sections results in some defects, but the qualitative behaviour persists.

5. Conclusion

It was demonstrated that the new moment method captures the polydisperse character of sprays as well as the dispersion of droplet velocity at one location. It was further observed that the splashing test-case with a low number of sections correctly predicts the qualitative behaviour of the physical phenomenon, a necessary condition for the success of this method. Currently, this moment method is applied to tests for evaporating droplets. These tests in one- and two-dimensional configurations and the detailed explanations of the theory and the numerical methods will be presented in the forthcoming publication [7].

References

[1] O. Desjardins, R.O. Fox, P. Villedieu, A quadrature-based moment method for dilute fluid-particle flows, J. Comp. Phys. 227 (4) (2008) 2514–2539.

[2] G. Dufour, P. Villedieu, The sectional method revisited for evaporating sprays, M2AN Math. Model. Numer. Anal. 39 (5) (2005) 931–936.

[3] A. Kaufmann, Towards Eulerian–Eulerian large eddy simulation of reactive two-phase flows, Ph.D. Thesis, Institute National Polytechnique de Toulouse, 2004.
[4] F. Laurent, M. Massot, Multi-fluid modelling of laminar polydisperse spray flames: origin, assumptions and comparison of sectional and sampling methods, Combust. Theory Modelling 5 (4) (2001) 537–572.
[5] F. Laurent, M. Massot, P. Villedieu, Eulerian multi-fluid modelling for the numerical simulation of coalescence in polydisperse dense liquid sprays, J. Comput. Phys. 194 (2) (2004) 505–543.
[6] M. Rüger, S. Hohmann, M. Sommerfeld, G. Kohnen, Euler/Lagrange calculations of turbulent sprays: the effect of droplet collisions and coalescence, Atomization Sprays 10 (1) (2000).
[7] L. Schneider, N. Le Lostec, P. Villedieu, A. Sadiki, A moment method for evaporation and splashing processes of polydisperse sprays, Int. J. Multiphase Flow, submitted for publication.
[8] F.A. Williams, Spray combustion and atomization, Phys. Fluids 1 (1958) 541–545.