International Journal of Heat and Fluid Flow 40 (2013) 151–164

Contents lists available at SciVerse ScienceDirect

International Journal of Heat and Fluid Flow

journal homepage: www.elsevier.com/locate/ijhff

Advanced statistics to improve the physical interpretation of atomization processes

Miguel R.O. Panão [a],*, Lucian Radu [b]

[a] IN+, Center for Innovation, Technology and Policy Research, Instituto Superior Técnico, Technical University of Lisbon, Portugal
[b] Faculty of Engineering, Catholic University of Portugal, Portugal

ARTICLE INFO

Article history:
Received 5 April 2012
Received in revised form 4 October 2012
Accepted 12 January 2013
Available online 11 February 2013

Keywords:
Statistical analysis
Finite mixture
Bayesian approach
Markov-chain Monte Carlo
Atomization
Multijet sprays

ABSTRACT

This paper reports an analysis of the physics of atomization processes using advanced statistical tools. Namely, finite mixtures of probability density functions, which best fitting is found using a Bayesian approach based on a Markov chain Monte Carlo (MCMC) algorithm. This approach takes into account eventual multimodality and heterogeneities in drop size distributions. Therefore, it provides information about the complete probability density function of multimodal drop size distributions and allows the identification of subgroups in the heterogeneous data. This allows improving the physical interpretation of atomization processes. Moreover, it also overcomes the limitations induced by analyzing the spray droplets characteristics through moments alone, particularly, the hindering of different natures of droplet formation. Finally, the method is applied to physically interpret a case-study based on multijet atomization processes.

1. Introduction

Statistical analysis is an essential tool for the characterization of atomization processes. Typically, fragmentation of the bulk liquid results in a broad and non-Gaussian drop size distribution, often dependent on the hydrodynamic mechanisms generating droplets. In the cases where more than one of these mechanisms are present, the drop size distribution characterizing the outcome of the atomization may be multimodal, expressing heterogeneities in drop size data. Multimodal drop size distributions may be due to measurement errors, or to the physical nature of the fragmentation process. In the context of the present work we focus on the later.

After having characterized multiple drop sizes resulting from an atomization process, the results are usually analyzed statistically in terms of drop size distributions and representative drop diameters, such as the arithmetic mean diameter based on number-weighted size distribution (d_{10}) as in most spray characterization experiments, the Sauter mean diameter, an average based on surface-weighted distributions (d_{32}) as in combustion applications, or the De Brouckere mean diameter based on volume-weighted distributions (d_{43}), as in spray cooling applications (Sowa, 1992). The purpose of using a representative drop diameter in the physical analysis of an atomization process is to replace the polydisperse drop size distribution with a monodisperse one, where each drop diameter is considered to have the same representative size. This latter is further used to analyze the effects of certain operating and environmental conditions upon the atomization process. Although this is a common approach on the characterization of atomization processes, its use to physically analyze cases where multimodality is observed in drop size distributions should be questioned and other statistical methods should be sought to provide a better interpretation of the results obtained. An example of this is when multimodality caused by multiple atomization mechanisms yields different characteristics within the same spray, namely, multiple polydispersions with different evaporative and combustion conditions.

Furthermore, in some modeling approaches for polydispersed drop sizes in sprays, the full nature of the spray is captured by its moments which are further transported using an Eulerian formulation. This apparently suggests the ability to reconstruct, for example, the number-distribution of drop sizes at any point in space and time in these modeling schemes (Beck and Watkins, 2003; Archambault, 2009). Therefore, it would be useful to have a method which would provide enough information enabling such reconstruction, as well as to retrieve physical information about the spray. In the literature, while drop-size distributions were obtained empirically by curve fitting the data collected for a wide range of experimental conditions; more recent approaches rely on the interpretation that the droplet generation process is non-deterministic (maximum entropy ME), or composed of deterministic and non-deterministic parts (discrete probability function DPF). The first interpretation (ME) states that the most likely droplet size distribution is the one that maximizes the entropy of the system (droplets in a spray), subjected to the constraints imposed by the conservation laws (mass, momentum and energy, including the

---

* Corresponding author.
E-mail address: mpanao@dem.ist.utl.pt (M.R.O. Panão).

0142-727X/$ - see front matter
http://dx.doi.org/10.1016/j.ijheatfluidflow.2013.01.012

Nomenclature

d or d_d	drop diameter (μm)
d_{10}	arithmetic mean diameter (μm)
d_{32}	Sauter mean diameter (μm)
d_{43}	average of volume-weighted drop size distribution (μm)
d_j	jet diameter (μm)
f	probability density function
$\bar{h}$	average liquid sheet thickness (μm)
k	wave number
K	number of components in the finite mixture of pdfs
N_j	number of jets
Oh_L	ligament Ohnesorge number
$p(y\|\mathcal{M}_K)$	marginal likelihood
S	allocation variable for data points
u_d	droplet axial velocity (m/s)
U_j	average jet velocity (m/s)
We_j	jet Weber number
y	general dataset

Greek symbols

γ	liquid surface tension (N/m)
η	weight of a probability distribution function
λ	wave length
μ	characteristic mean
ξ	ligament diameter (μm)
ρ	liquid density (kg/m^3)
σ	characteristic standard deviation
θ	impingement jet angle
ω	liquid sheet wave growth rate

Subscripts

G	surrounding gaseous environment
L	liquid
max	maximum
mix	mixture
N	Normal distribution

Acronyms

C	capillary
KH	Kelvin–Helmholtz
LFS	Leading Fron of the Spray period
MCMC	Markov-chain Monte Carlo
ML	Maximum Likelihood
pdf	probability density function
SS	Steady Spray period
ST	Spray Tail period

surface and kinetic components). The second interpretation (DPF) predicts droplets to be distributed around a mean size determined by a breakup model subjected to initial conditions which fluctuate in a non-deterministic manner, described by a continuous probability density function, (see the review by Babinsky and Sojka (2002)). In both cases, the main concern is how well can a discrete drop size distribution be described mathematically, but in this paper, the question is whether it is possible to retrieve any physical information of the atomization process itself through the statistical methodology used to describe it. What is the nature of droplet formation? Does it involve a single or multiple breakup meachanisms? Is is possible to distinguish the characteristics of droplets produced by different atomization mechanisms?

This work follows a previous one (Panão et al., 2010) and the objective is attempting an answer to these questions using the known advanced statistical tool of finite mixture of probability distribution functions (p.d.f.). This finite mixture is nothing more than a weighted linear combination of several mathematical pdfs, for example, Normal, Log-Normal, Gamma or others, which best describes a discrete probability distribution of any acquired quantity experimentally measured. Although this tool is in line with the empirical method, its scope is not restricted to determine a mathematical form that fits the experimental data collected (Babinsky and Sojka, 2002), but also overcome the limitations of using drop size distribution moments alone to describe the characteristics of a spray, and explore the applicability of using finite mixtures of probability density functions to improve the accuracy in that description, as well as the physical interpretation of atomization processes. In this work, it is shown the fundamentals of how finite mixture distributions can better capture some specific or hidden properties of droplets size data such as unobserved heterogeneities, which is useful to numerical modeling. In order to find the best mixture fitting data, a Bayesian approach based on a Markov chain Monte Carlo (MCMC) algorithm is used. This method has been recently applied to the characteristics of secondary atomization resulting from the spray impact onto a flat surface under cross-flow (Panão et al., 2012d). For the first time, the characteristic size of droplets produced by a mechanism known as film stripping has been identified due to the application of this statistical tool. Also, current ongoing developments are being investigated to extend this advanced statistical analysis to improve the interpretation of vortical flows as described in Barata et al. (2009). Our experience shows that, as long as a certain flow can be described through statistics with discrete probability distributions of a certain quantity, the method here explored of finite mixtures of probability density functions can be applied.

Furthermore, this unsupervised Bayesian learning is applied to the physical interpretation of a case-study associated with multijet atomization phenomena, which can be used in several kinds of applications, from macroscale showers (Panão et al., 2012b) to microscale spray cooling (Panão et al., 2012a,c) and combustion engines (Durst, 2010). A multijet atomization consists of a liquid disintegration process which generates droplets of polydispersed sizes through the simultaneous impact of N_j cylindrical jets. Most experimental works performed in this atomization strategy are dedicated to the impact of two jets, and studies on a spray produced by the impact of more than two are scarce. In a previous work (Panão et al., 2012e) it has been observed that sprays formed with more than two jets generate tridimensional structures with periodic patterns associated with the formation of ligaments and further disruption into droplets. The characteristics of these droplets have been measured for several points in a measurement grid using a Phase–Doppler Interferometer which details on the optical configuration can be found in Panão et al. (2012e). In this work, the Bayesian approach used to physically interpret liquid atomization considers the entire spray, i.e. the measurement data includes all the information collected within the measurement grid established for each atomizer.

2. Statistical method

Although the Bayesian approach using an MCMC algorithm can be applied to any known kind of mathematical probability distribution function, in this work, we assume that a drop size distribution can be described by a mixture of Log-Normal distributions with an unknown number of components. In fact, it has been re-