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Spray characterization: numerical prediction of Sauter mean diameter and droplet size distribution

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A simplified equation of the Nukiyama–Tanasawa type for droplet size distribution in sprays is obtained from the synergetic concept of entropy information, assuming spherical droplets and zero and infinity as their limit sizes. The introduction of Sauter mean diameter (SMD) definition in that equation yields a new distribution function dependent solely on SMD, which is calculated from available correlations for pressure-jet and pre-filming airblast atomizers. For plain-jet airblast atomizers a new and dimensionally consistent correlation is determined. Several droplet size distributions are then predicted. Experimental data are compared with predictions of SMD; the agreement is satisfactory. *Copyright © 1996 Elsevier Science Ltd.*

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Interest in the size distributions of droplets in fuel nozzle sprays has increased during the past few years. This is partly due to the combined effects of relatively low prices of residual fuel oils and the growing concern about pollutant emissions. Undesired emissions together with particulate formation in spray combustion are influenced to a significant extent by spray quality. Moreover, present demands in industrial processes for better energy efficiency and for environmental control have emphasized the need for better understanding of all types of thermal and pollutant emission processes. The effect of fouling on furnace heat transfer, which is influenced by the spray quality, is one of the many factors that requires closer attention.

Over a comparable period of time there has been a vastly increased interest in mathematical modelling on the part of combustion equipment manufacturers, as a means of determining design improvements. Mathematical models require a precise specification of the geometry and all other boundary conditions as a basis for obtaining predictions. Existing models applicable to two-phase flows in oil-fired combustors make no attempt to predict spray characteristics by initiating calculations of processes within the atomizer gun itself. Rather, they rely on a specification of the droplet size distributions (DSD), trajectories and velocities over a plane near the atomizer exit. An extensive and difficult measurement programme would be required to achieve this specification, a very demanding task which would be effected for every atomizer for all operating conditions. Presently, the only practicable approach is to develop numerical methods able to characterize the sprays from different atomizer types. These methods should have an acceptable accuracy so that useful predictions can be obtained for a realistic range of operating conditions.

The droplet size distribution is frequently characterized by its Sauter mean diameter. In turn, the SMD is influenced by the properties of the atomized and atomizing fluids and by the nozzle design and operating conditions; see, for example, Chigier[1] and Lefebvre[2]. A semi-empirical correlation, permitting the calculation of SMD in terms of those factors, is reported by Lefebvre[3] and Wang and Lefebvre[4]. This correlation is obtained from basic considerations about the physical processes involved in pressure-swirl atomization and about dimensional analysis. Satisfactory agreement with experimental data is demonstrated. In the present work the previous correlation is used to predict SMD for pressure-jet atomizers. The data reported by Jasuja[5] are added to obtain wider validation and improved tuning of the constants appearing in the above-mentioned correlation.

According to Lefebvre[2], the twin-fluid atomization process is more extensively used in practice. Studies of pre-filming airblast atomizers were initiated by Wigg[6] and thoroughly continued by Rizkalla and Lefebvre[7,8]. The latter examined the effects of changing both fuel and atomizing-air properties on the mean drop size. The authors proposed a useful correlation based on a combination of dimensional and physical analysis of the atomization process. This correlation, with tuned constants obtained by Jasuja[5], is used here to predict the SMD for pre-filming airblast atomizers, and the results are compared with a range of experimental data.

Studies of plain-jet atomizers are reported by Lorenzetto and Lefebvre[9], Jasuja[5], Shaw and Jasuja[10] and Carvalho *et al.*[11]. Jasuja[5] determined an interesting correlation for the SMD which gives rewarding fits to the experimental data but which is dimensionally inconsistent. The present work builds on these previous studies. Following the work of Carvalho *et al.*[11], a modified correlation for SMD is derived and the predictions of this are tested against the data reported in that work.

MATHEMATICAL FORMULATION OF DROPLET SIZE DISTRIBUTION

The droplet size distribution in sprays is the crucial parameter needed for the fundamental analysis of the transport of mass, momentum and heat in engineering systems. Moreover, that parameter determines the quality of the spray and consequently influences to a significant extent the processes of fouling and undesired emissions in oil combustion. Various distribution functions have been used to fit the existing experimental data. The most commonly used functions are the Rosin–Rammler and Nukiyama–Tanasawa, plus modified formulations such as the upper-limit, log–normal and chi-squared functions. In the present paper, attention is confined to the Nukiyama-Tanasawa function[12]:

$$\frac{dN}{dD} = BD^p \exp(-CD^q) \tag{1}$$

where B, C, p and q are adjustable constants, D is the droplet diameter and N is the normalized number distribution. In Equation (1), dN stands for the percentage of the total number of droplets with a diameter contained in the interval $[D, D + dD]$.

An important task for researchers concerned with engineering application of sprays is the tuning of the adjustable parameters with the conditions of the atomizing system. Those parameters are the viscosity and surface tension of the liquid, mass flow rates, atomizer design, etc. Li and Tankin[13] derived an equation for the droplet size distribution, assuming spherical droplets with sizes varying from zero to infinity. This equation is characterized by the total number of droplets produced per unit time by the atomizer. In this work a similar equation is derived, but the characterizing parameter is the SMD rather than the number of droplets produced per unit time. Knowledge of the SMD is now the only necessary input required for the calculation of the droplet size distribution at the atomizer exit plane.

Following Li and Tankin[13], the DSD is obtained by solving a non-linear optimization problem, that is, by finding the extreme value of Equation (2):

$$S = -K \sum_i P_i \ln P_i \tag{2}$$

where S is the information entropy, the name used when the information concept is applied to problems in physics and engineering. In this equation K is a constant and P_i is the probability of the occurrence of a certain result, in terms of number fraction. In the present work, that result represents the existence of a droplet within the spray with a volume V_i and density ρ_i.

The following physical and mathematical constraints must be obeyed:

(i) the sum of all probabilities must be unity:

$$\sum_i P_i = 1 \tag{3}$$

(ii) the mass flow of sprayed liquid must be equal to the mass of all droplets produced per unit time:

$$\sum_i P_i V_i \rho_i \dot{n} = \dot{m}_L \tag{4}$$

where $\dot{n}$ is the total number of droplets produced per unit time and $\dot{m}_L$ is the liquid mass flux. The solution of this optimization problem is obtained by using Lagrangian multipliers. Moreover, the assumption is made that the droplets are spherical, with zero and infinity as the limit values of their size. Finally, converting the variables in the resulting equations from the discrete case to the continuous case leads to the following distribution function (see Li and Tankin[13] for details):

$$\frac{dN}{dD} = \frac{\pi}{2} D^2 \frac{\rho_L \dot{n}}{\dot{m}_L} \exp\left(-\frac{\pi \rho_L \dot{n}}{6 \dot{m}_L} D^3\right) \tag{5}$$

where ρ_L is the liquid density.

Introducing the definition of SMD:

$$\mathrm{SMD} = \frac{\int_0^\infty D^3 \, dN}{\int_0^\infty D^2 \, dN} \tag{6}$$

and substituting Equation (5) into Equation (6), the SMD becomes:

$$\mathrm{SMD} = \left(\frac{6}{\pi}\right)^{1/3} \frac{\Gamma(2)}{\Gamma(\frac{5}{3})} \left[\frac{\dot{m}_L}{\rho_L \dot{n}}\right] \tag{7}$$

where $\Gamma(n)$ is the statistical gamma function, defined as:

$$\Gamma(n) = \int_0^\infty e^{-x} x^{n-1} \, dx \tag{8}$$

Combining Equations (5) and (7), the final expression for the droplet size distribution, as a function of SMD, becomes:

$$dN = \frac{3}{[\Gamma(\frac{5}{3})]^3} \left(\frac{D}{\mathrm{SMD}}\right)^2 \exp\left\{-\frac{1}{[\Gamma(\frac{5}{3})]^3} \left(\frac{D}{\mathrm{SMD}}\right)^3\right\} \frac{dD}{\mathrm{SMD}} \tag{9}$$

In terms of volume fraction, the preceding equation for spherical droplets becomes:

$$dV = \frac{3}{[\Gamma(\frac{5}{3})]^6} \left(\frac{D}{\mathrm{SMD}}\right)^5 \exp\left\{-\frac{1}{[\Gamma(\frac{5}{3})]^3} \left(\frac{D}{\mathrm{SMD}}\right)^3\right\} \frac{dD}{\mathrm{SMD}} \tag{10}$$

Hence the SMD is the only parameter necessary to calculate the droplet size distribution, given by Equations (9) and (10).

EQUATIONS FOR MEAN DROPLET SIZE FOR DIFFERENT ATOMIZERS

The prediction of SMD for different types of atomizers is still based on semi-empirical correlations, obtained from experimental data and physical and dimensional analysis of the atomizing process. Several equations have so far been proposed in the literature (see for example refs 1–11).

The correlations used in the present work to predict the SMD for pressure-jet and pre-filming airblast atomizers, which were included in the code developed, were taken from the literature. For SMD from plain-jet airblast atomizers a new and dimensionally consistent correlation is obtained here and the predictions are compared with experimental data.

SMD correlation for pressure-jet atomizers

According to Lefebvre[3] and owing to the complexity of the various physical phenomena involved in pressure-swirl nozzles, the study of atomization has been pursued principally by empirical methods. These studies yielded correlations for mean droplet sizes of the form $\mathrm{SMD} \propto \sigma^a, V^b, \dot{m}_L^c, \Delta p_L^d$. The correlation presented in this work was obtained by Lefebvre[3] and Wang and Lefebvre[4] and takes into account the basic mechanisms involved in pressure-swirl atomization. This process is mainly a result of two kinds of acting forces: aerodynamic forces caused by the relative velocity between liquid and the surrounding gas, and hydrodynamic forces caused by the turbulence or other disruptive forces within the liquid itself. Aerodynamic forces develop waves on the liquid surface and consequently produce unstable ligaments that eventually disintegrate into droplets on any increase in the relative velocity.

Because of this complexity, it is more convenient to consider droplet formation as a two-stage process. The first stage represents the generation of surface instabilities due to the combined effects of hydrodynamic and aerodynamic forces, while the second stage is the conversion of surface protuberances into ligaments and then drops. This approximation is undoubtedly a gross oversimplification of the actual mechanisms involved, but it allows the postulation of an equation $\mathrm{SMD} = \mathrm{SMD}_1 + \mathrm{SMD}_2$. In this equation SMD_1 depends partly on the Reynolds number, which provides a measure of the disruptive forces present within the liquid sheet. SMD_1 also depends on the Weber number, which governs the growth rate of perturbations into projections large enough to break off and form ligaments. SMD_2 represents the last stage of atomization. In this stage the high relative velocity induced at the liquid–air interface causes the surface protuberances generated in the first stage to become detached and break down into ligaments and then drops. According to Wang and Lefebvre[4] the SMD is given by:

$$\mathrm{SMD} = A\left[\frac{\sigma^{0.5}\mu_L}{\rho_A^{0.5}\Delta p_L}\right]^{0.5}[t\cos\theta]^{0.25} + B\left[\frac{\sigma\rho_L}{\rho_A\Delta p_L}\right]^{0.25}[t\cos\theta]^{0.75} \quad (11)$$

where σ is the liquid surface tension, μ_L is the liquid viscosity, ρ_A is the air density, ρ_L is the liquid density, Δp_L is the injection pressure differential across the nozzle, θ is the half spray angle and t is the film thickness, given by

$$t = 2.7\left(\frac{d_0\,\mathrm{FN}\,\mu_L}{\sqrt{\Delta p_L\rho_L}}\right)^{0.2}$$

where d_0 is the discharge orifice diameter and FN is the nozzle flow number defined by

$$\mathrm{FN} = \frac{\dot{m}_L}{\sqrt{\Delta p_L\rho_L}}$$

In this work, the constants A and B were evaluated from experimental results of Lefebvre[3], Wang and Lefebvre[4] and Jasuja[5] and have the expressions:

$$A = 2.11[\cos 2(\theta - 30)]^{2.25}\left(\frac{3.4\times10^{-4}}{d_0}\right)^{0.4} \quad (12)$$

$$B = 0.635[\cos 2(\theta - 30)]^{2.25}\left(\frac{3.4\times10^{-4}}{d_0}\right)^{0.2} \quad (13)$$

SMD correlations for airblast atomizers

An alternative to pressure-jet atomization is to expose the relatively slow-moving liquid to a high-velocity air stream: airblast atomization. There are two types of airblast atomizer. In pre-filming airblast atomizers, the liquid is spread into a thin continuous sheet of uniform minimum-possible thickness, and is then exposed on both sides to air at the highest-possible velocity. In plain-jet airblast atomizers the liquid is not transformed into a thin sheet but instead is injected as discrete round jets into a high-velocity coaxial air flow. According to Lefebvre[2], the consistency of the experimental findings in regard to the effects of the main liquid and air stream variables on mean droplet size, which is such a notable feature of most published data on pre-filming airblast atomizers, is less apparent with plain-jet atomizers.

In the present work the semi-empirical correlation of Rizkalla and Lefebvre[8], with constants tuned by Jasuja[5], for pre-filming airblast atomizers is used to predict the SMD:

$$\mathrm{SMD} = 10^{-3}\left[\frac{\sqrt{\sigma\rho_L}}{\rho_A V_A}\right]\left(1+\frac{1}{\mathrm{AFR}}\right)^{0.5} + 6\times10^{-5}\left[\frac{\mu_L^2}{\sigma\rho_A}\right]^{0.425}\left(1+\frac{1}{\mathrm{AFR}}\right)^{0.5} \quad (14)$$

where σ, μ_L, ρ_A and ρ_L have the same meanings as in Equation (11), V_A is the air velocity and AFR is the air/fuel ratio.

The correlation proposed by Jasuja[5] for plain-jet airblast atomizers was tested against the experimental data obtained by Carvalho *et al.*[11]. The results show that this correlation for SMD, which is dimensionally inconsistent, does not fit those data. Indeed, the predicted values are about ten times the measured values. In the present work, an improved and dimensionally consistent correlation for this type of atomizer is obtained, based on the data of Carvalho *et al.*[11] and Lorenzetto and Lefebvre[9], together with the dimensional analysis described below.

As described by Lefebvre[2], for liquids of low viscosity such as water and kerosene, the main factors governing SMD are liquid surface tension, air density and air velocity. On the other hand, for liquids of high viscosity the effects of air properties are less significant, and SMD becomes more dependent on the liquid properties, especially viscosity. As in the case of pressure-jet atomization, it is possible for plain-jet atomizers to postulate the equation $\mathrm{SMD} = \mathrm{SMD}_1 + \mathrm{SMD}_2$. In this equation SMD_1 (determinant in atomization of liquids with low viscosity) is governed by, among other non-dimensional parameters, the Weber number. This

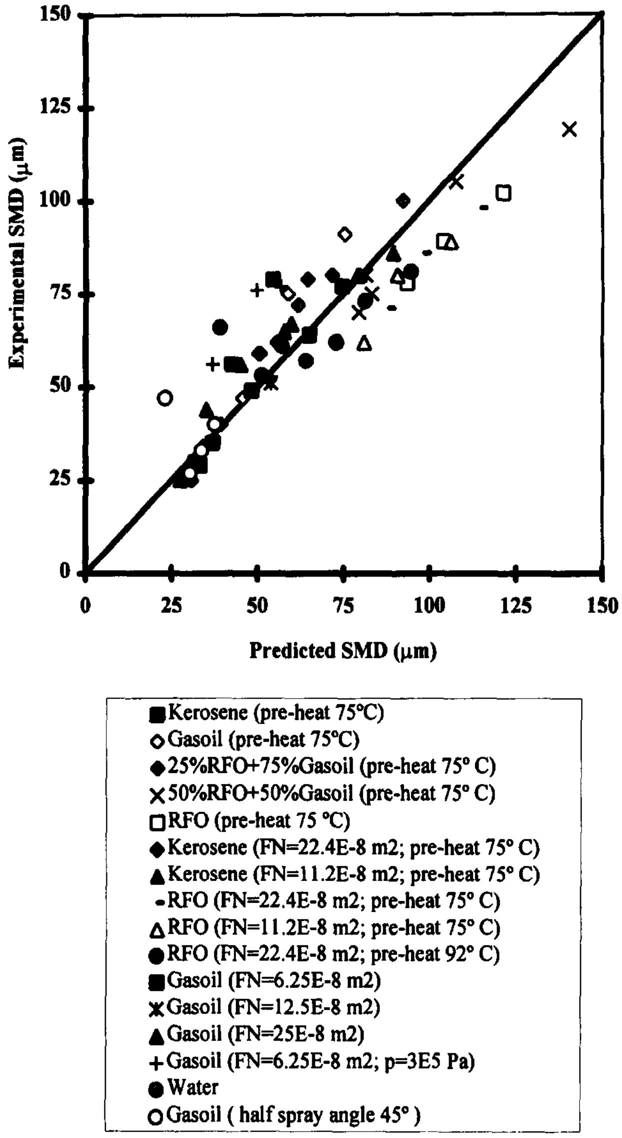

Figure 1 Pressure-jet atomizer: comparison of predicted and experimental SMD (data from refs 3–5)

non-dimensional parameter represents the ratio of the disrupting aerodynamic forces to the consolidating surface tension forces: $We = \rho_A V_A^2 d_0/\sigma$. For liquids possessing higher viscosity, it is necessary to account for a different mechanism represented by SMD_2. This parameter is found to be dependent on the product of the characteristic dimension of the atomizer and on the Z number, obtained as the ratio of the square root of the Weber number to the Reynolds number ($Re = \rho_L V_R d_0/\mu_L$, where V_R is the relative velocity, with a value near the air velocity). The previous description yields:

$$\frac{\mathrm{SMD}}{d_0} \propto F\left(We, Re, \mathrm{AFR}, \frac{\rho_L}{\rho_A}\right) \quad (15)$$

$$\frac{\mathrm{SMD}_1}{d_0} \propto \frac{1}{We}, \frac{Re}{We}, \mathrm{AFR}, \frac{\rho_L}{\rho_A} \quad (16)$$

$$\frac{\mathrm{SMD}_2}{d_0} \propto \frac{1}{Re}, \frac{1}{We}, \mathrm{AFR}, \frac{\rho_L}{\rho_A} \quad (17)$$

Further dimensional analysis, together with the experimental data, yields the following equation for SMD of plain-jet airblast atomizers:

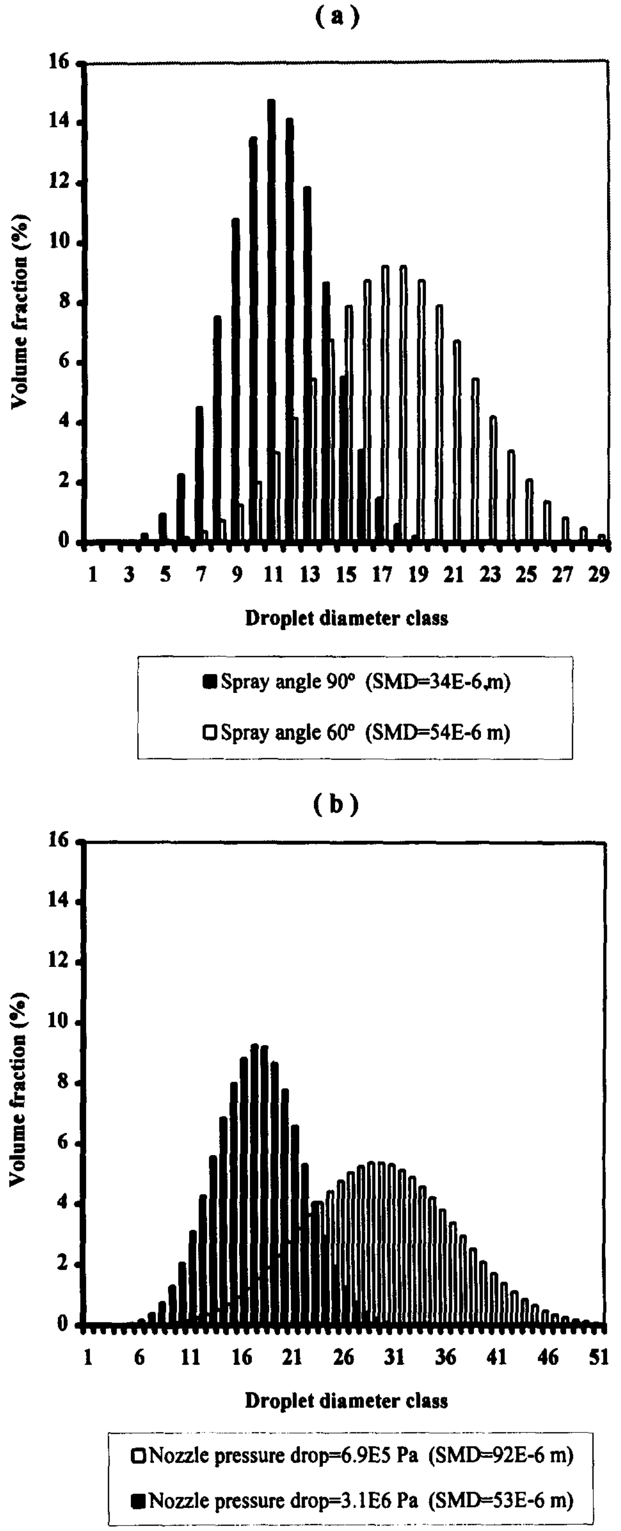

Figure 2 Droplet size distributions for pressure-jet atomizers: a, spray angle effect (diesel oil, $\mathrm{FN} = 1.25 \times 10^{-7}\,\mathrm{m}^2, \Delta p_L = 6.9 \times 10^5\,\mathrm{Pa}$); b, nozzle pressure drop effect (75% gas oil + 25% RFO, $\mathrm{FN} = 3.58 \times 10^{-7}\,\mathrm{m}^2, \theta = 30°$)

$$\mathrm{SMD} = 1.58 \times 10^3 \left[\frac{\sigma}{\rho_A V_A^2 d_0}\right]^{0.5} d_0 \left[\frac{\sigma}{\mu_L V_A}\right]^{0.55} \left(\frac{\rho_L}{\rho_A}\right)^{-1} \times \left[1 + \frac{1}{\mathrm{AFR}}\right]^{0.5} + 166 \left[\frac{\mu_L}{\rho_L d_0 V_A}\right]^{1.1} \times \left[\frac{\sigma}{\rho_A V_A^2 d_0}\right]^{0.2} d_0 \left(\frac{\rho_L}{\rho_A}\right)^{0.35} \left[1 + \frac{1}{\mathrm{AFR}}\right]^{-0.48} \quad (18)$$

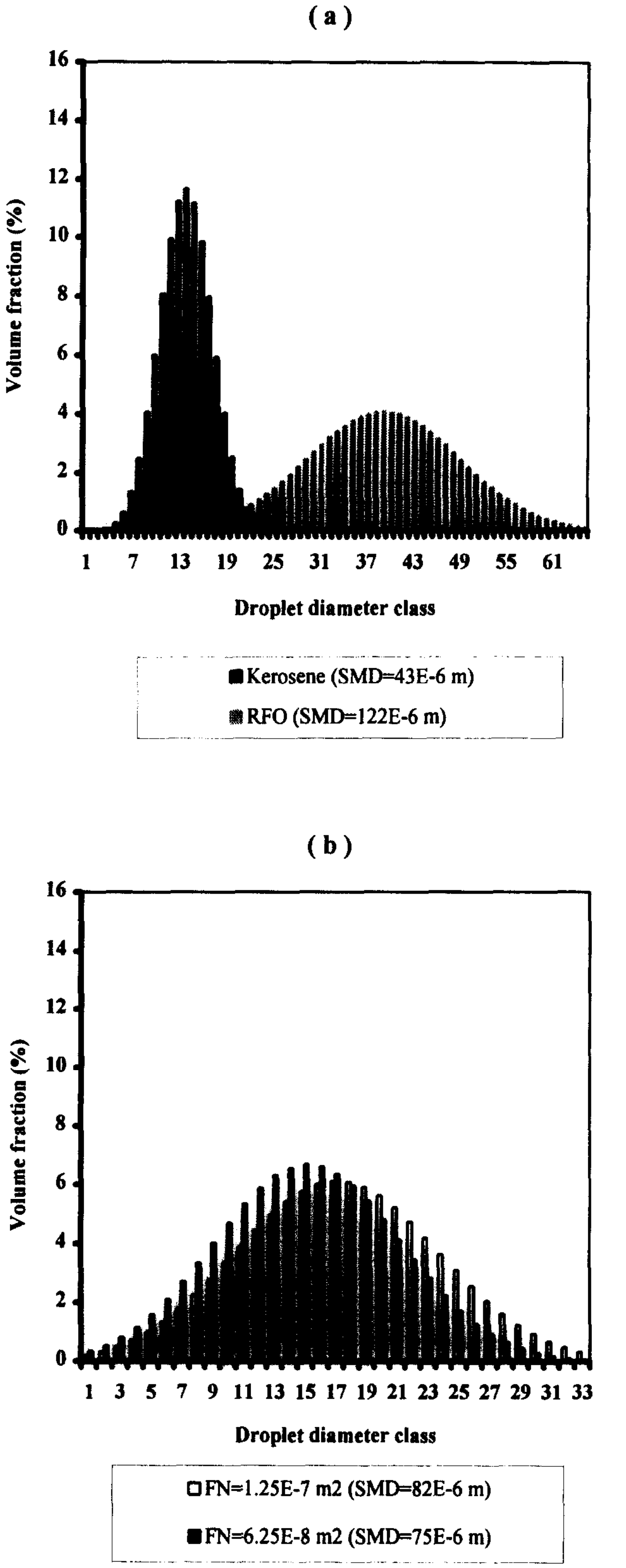

Figure 3 Droplet size distributions for pressure-jet atomizers: a, effect of fuel type (kerosene and RFO, $FN = 3.58 \times 10^{-7}\,m^2$, $\Delta p_L = 13.9 \times 10^5$ Pa, $\theta = 30°$); b, effect of FN (gas oil, $\Delta p_L = 6.9 \times 10^5$ Pa, $\theta = 30°$)

where σ, μ_L, ρ_A, ρ_L, V_A, AFR and d_0 assume the same meanings as in Equations (11) and (14).

RESULTS AND DISCUSSION

Pressure-jet atomizers

The predicted values of SMD for pressure-jet atomizers, using Equations (11) to (13), are depicted in *Figure 1* in comparison with the respective experimental results obtained by Lefebvre[3], Wang and Lefebvre[4] and Jasuja[5]. As can be observed, the SMD predictions are in good agreement with the experimental values, although some discrepancies can be noted. Nevertheless, the possibility of using such kind of correlation, for both pressure-jet and airblast atomizers, offers the great advantage of allowing fairly good predictions of SMD and DSD. This can avoid the need for extensive and difficult measurement programmes to obtain the initial conditions for spray calculations.

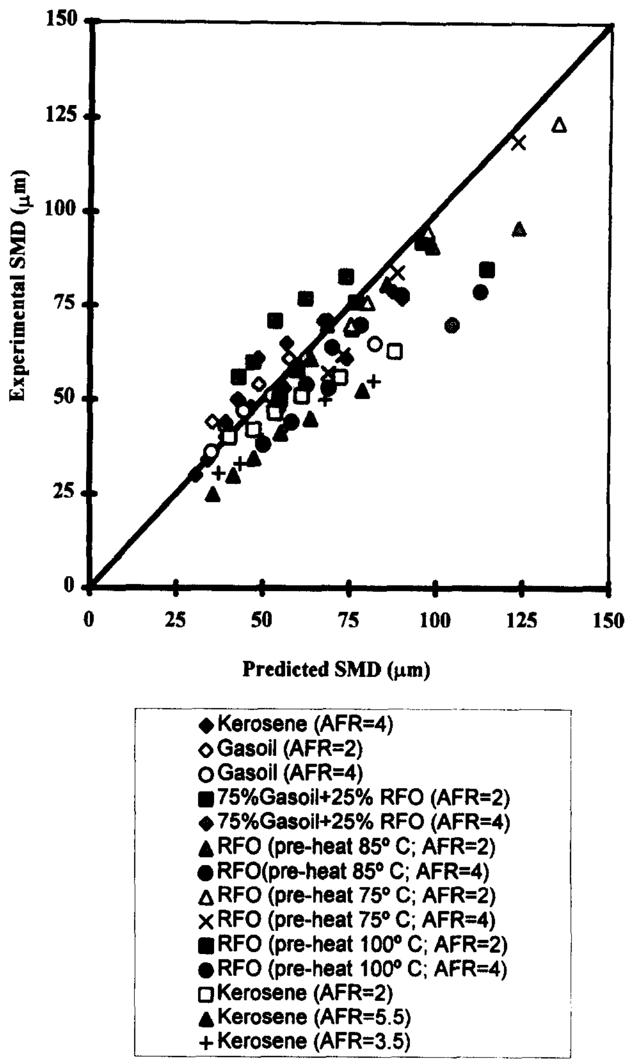

Figure 4 Pre-filming airblast atomizer: comparison of predicted and experimental SMD (data from refs 5 and 8)

Several DSDs are depicted in *Figures 2* and *3*, as a function of the diameter classes chosen to discretize the distribution. Each class has a range of 2.5 μm, the first class beginning at 0. *Figure 2a* shows a comparison of different distributions with the spray angle varied, while *Figure 2b* shows the DSDs for two different values of nozzle pressure drop. An increase in spray angle improves the atomization quality: the DSD in *Figure 2a* occurs at smaller diameters and is more uniform (i.e. with fewer classes around the SMD). This is due to the reduction of the liquid sheet thickness, with a consequent decrease in the SMD, when the spray angle is increased. Again, a higher injection pressure differential across the nozzle increases the Reynolds number—a measure of disruptive forces. Therefore, more favourable

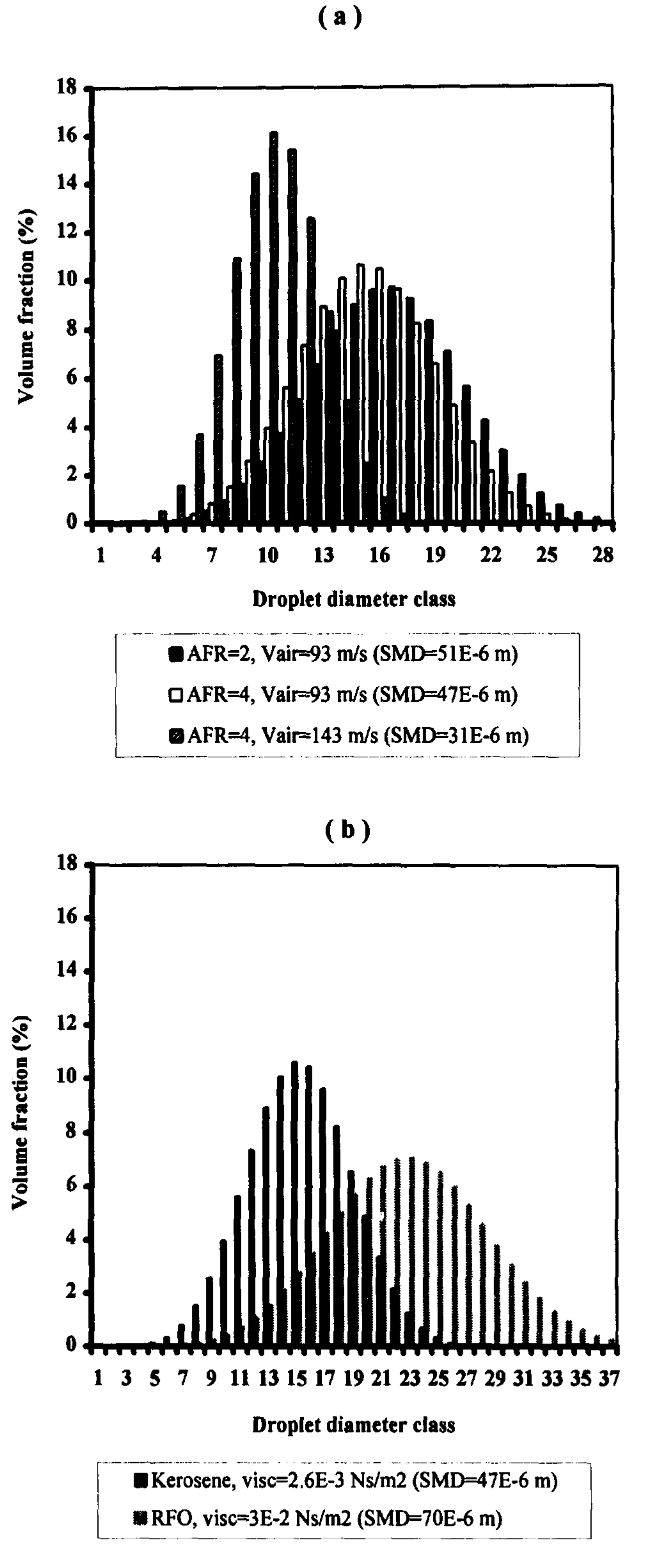

Figure 5 Droplet size distributions for pre-filming airblast atomizers: a, air/fuel ratio and air velocity effects (kerosene); b, fuel viscosity effect (AFR = 4, $V_A = 93\,\mathrm{m\,s^{-1}}$)

distributions are produced, with smaller diameters of droplets, as depicted in *Figure 2b*, where the distribution is nearer the *y*-axis.

The DSDs of two different fuels, kerosene and residual fuel oil (RFO), are compared in *Figure 3a*, while *Figure 3b* contains distributions for two different atomizers characterized by their flow numbers (FN). Kerosene, due to its low surface tension, viscosity and density, responsible for cohesion forces, exhibits a DSD much more favourable than that for RFO (see *Figure 3a*). Conversely, as the liquid pressure drop is sufficiently high—0.7 MPa—the atomization quality, as can be observed in *Figure 3b*, is not very sensitive to the atomizer flow number (which gives a measure of the size of the atomizer), as already verified by Lefebvre[3]. Indeed, the improvement obtained in the spray quality is markedly inferior to that resulting from changing other parameters.

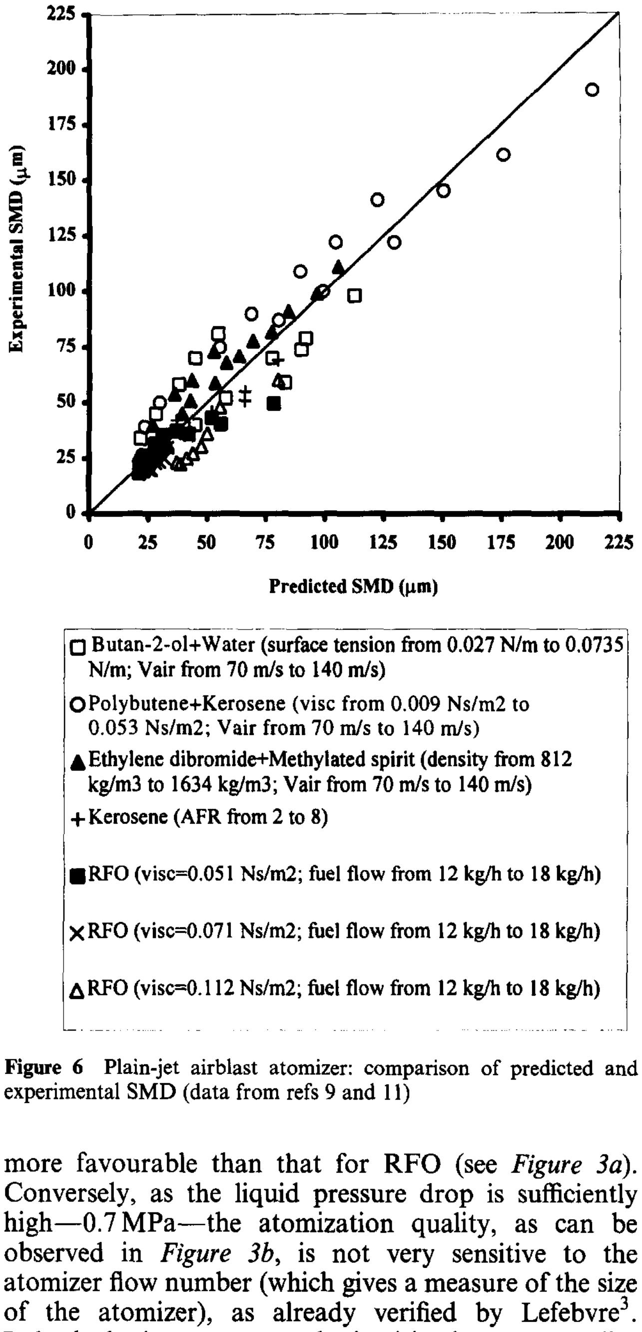

Figure 6 Plain-jet airblast atomizer: comparison of predicted and experimental SMD (data from refs 9 and 11)

Pre-filming airblast atomizers

The values of SMD predicted for pre-filming airblast atomizers, using Equation (14), are displayed in *Figure 4* in comparison with the corresponding experimental results obtained by Jasuja[5] and Rizkalla and Lefebvre[8]. Fairly good agreement with the experimental values can be observed, although there are some discrepancies.

Figure 5 shows the DSD as a function of the previously defined diameter classes. *Figure 5a* compares three different distributions, with the air/fuel ratio (AFR) and the air velocity varied, while *Figure 5b* shows DSDs for two different fuels, kerosene and RFO. It can be noticed that an increase in AFR markedly improves the atomization quality (*Figure 5a*), by producing more uniform distributions with lower SMD values. This is due to the fact that higher air flow rates promote

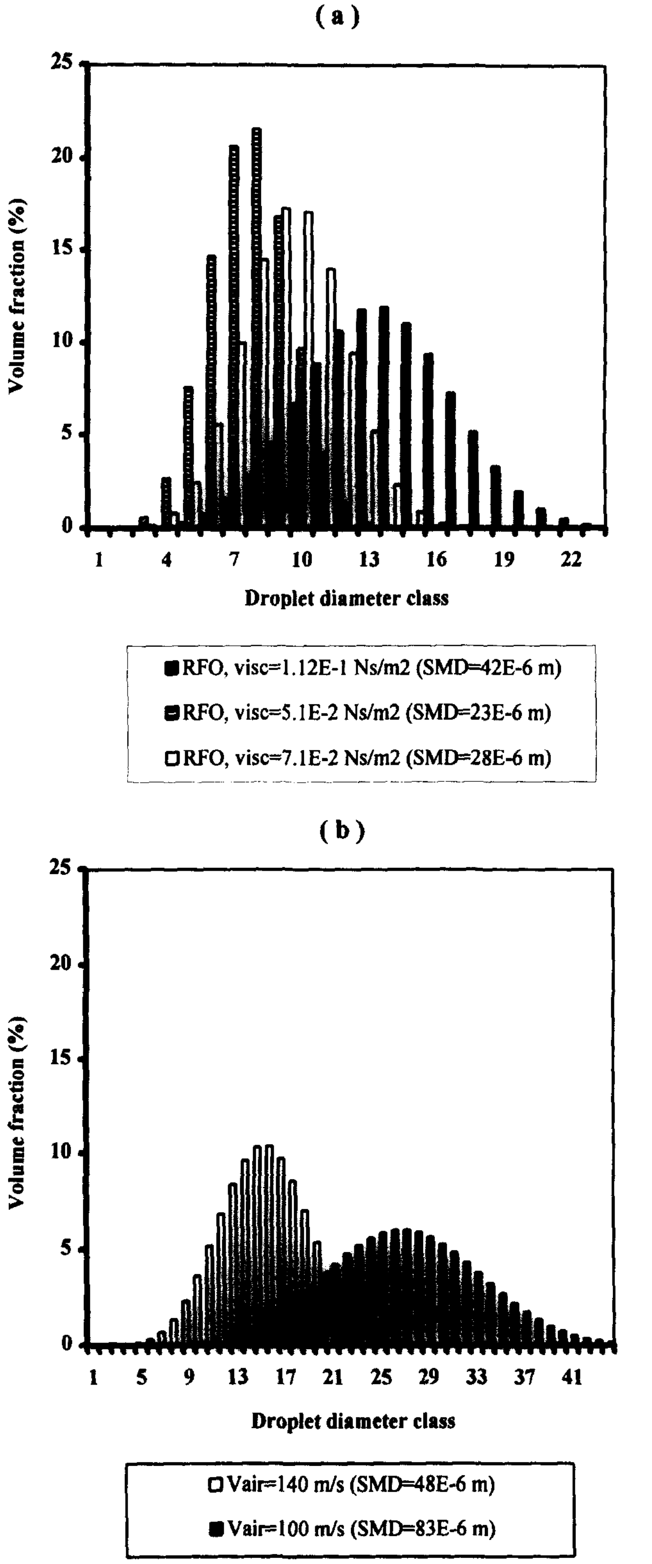

Figure 7 Droplet size distributions for plain-jet airblast atomizers: a, fuel viscosity effect ($\dot{m}_L = 0.005\,kg\,s^{-1}$, $V_A = 189\,m\,s^{-1}$, $d_0 = 2.25\,mm$); b, air velocity effect ($\dot{m}_L = 0.0015\,kg\,s^{-1}$, $d_0 = 0.794\,mm$)

more efficient disintegration mechanisms within the liquid, by the growth of interface aerodynamic forces. For the same reason, *Figure 5a* shows that a higher atomizing air velocity produces a better DSD. Paralleling the behaviour displayed in pressure-jet atomizers, in pre-filming airblast atomizers kerosene exhibits much better distributions than RFO, as shown in *Figure 5b*. This confirms other authors' research conclusion that fuels with lower surface tension, density and especially viscosity yield sprays of higher quality.

Plain-jet airblast atomizers

Figure 6 shows a comparison between measured values of SMD obtained by Lorenzetto and Lefebvre[9] and Carvalho *et al.*[11] and the corresponding predicted values for plain-jet airblast atomizers, using the new correlation defined by Equation (18). The agreement is very satisfactory. This equation appears to offer distinct advantages over existing equations in regard to improved correlation of SMD data obtained in the literature for plain-jet airblast atomizers.

Figure 7 shows some DSDs as a function of the diameter classes. *Figure 7a* compares three different distributions with the viscosity of RFO varied, while *Figure 7b* contains DSDs for two different values of atomizing air velocity. An increase in liquid viscosity impairs the spray quality—see *Figure 7a*—as already observed in other types of atomizers. This is due to the fact that higher viscosity impedes the disintegration mechanisms within the liquid, as viscosity has a cohesive effect. Owing to the dependence of the superficial aerodynamic disruptive forces on air velocity, a higher atomizing air velocity promotes a better DSD, as depicted in *Figure 7b*.

CONCLUSIONS

A new and dimensionally consistent equation for the prediction of the SMD of twin-fluid airblast atomizers has been determined from basic considerations of the physical processes involved in air-assisted atomization. Those processes involve competition between aerodynamic disruptive forces and the counter-disruptive forces of surface tension and viscosity. This equation appears to offer distinct advantages over existing equations in regard to improved correlation of SMD data obtained in the literature for plain-jet airblast atomizers.

The use of the above equation for plain-jet airblast atomizers, together with those for pressure-jet and pre-filming airblast atomizers obtained from the literature, enables droplet size distributions to be predicted for liquid sprays. The DSD is a crucial parameter for two-phase flow predictions. The numerical code developed for the above-mentioned predictions, where the droplet size distribution is calculated with recourse to an analytically derived equation of the Nukiyama–Tanasawa type, is a powerful tool for engineering design of atomizers. Indeed, this procedure can avoid the need for extensive and difficult measurement programmes to obtain the initial conditions for numerical spray calculations.

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