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Influence of the Spread/Splash Transition Criteria in the Spray Impingement Modeling

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Abstract: The present paper reports a numerical study of a spray impinging on a surface through a crossflow. This work is intended to study the influence of the spread/splash transition criteria in the modeling of the spray impingement phenomenon. Several experimental correlations available in the literature are inserted in the same base model and the results are tested against experimental data. It can be concluded that the employment of an accurate transition criteria can improve the quality of the results.

Key words: Spray impingement, droplets-wall interaction, transition criteria, splash regime.

1. Introduction

The present work is devoted to the turbulent dispersion and spray impingement on a solid surface, which have major importance in combustion systems performance and optimization. Over the last decades, the spray study has generated great interests among the scientific community due to its application in industry, agriculture, science and medical purposes. During these years, scientists have been studying intensively spray properties always trying to achieve the best model, even for comparison, for each particular application. The spray combustion application has been a concern due to the pollutant emission limitations which affect the society nowadays. Therefore, efforts are being made in order to improve direct injection gasoline engine performance lowering NOx (nitrogen oxide) emissions and other pollutants from aircraft gas turbine engines, such as carbon oxide, carbon monoxide, soot and unburned hydrocarbons [1]. Spray optimum conditions for better combustor performance are not yet completely clear but it is known that it affects combustion stability, efficiency and pollutant formation. Aerodynamic efficiency of redistribution, fuel and air mixing in combustion chamber and the desired temperature level and temperature profile are also important factors for combustion quality and generated emissions levels. Due to the uncertainty of the most favorable spray conditions to optimize the combustor performance all empirical findings have been difficult to generalize or extrapolate. Therefore, prediction methods based on a theoretical basis are needed and expected, in the hope of achieving correlations for use in the numerical simulations of injection and combustion phenomena inside engines.

Spray-wall interaction is considered to be an important phenomenon in IC (internal combustion) engines. In an attempt to achieve desirable air-fuel mixing and combustion, the fuel is sprayed either in the carburetor, port, pre-chamber, or directly in the cylinder. In all the designs, the fuel spray may impinge on engine surfaces before vaporization and mixing are complete. The spray impingement phenomenon has been shown to influence engine performance and emissions in both CI (compression ignited) and engines SI (spark ignited). A better understanding of these interactions between the liquid and induction surfaces will help in designing injection systems and control strategies to improve engine performance and to control emissions.

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The spray-wall interactions are difficult to analyze in operating engines because of the problems of access and despite useful information can be obtained by, for example, photographic techniques in specially adapted engines (e.g., as in Ref. [2]), the details of the data that can be obtained in this way are very limited, and it is difficult to alter the test conditions. For these reasons, most of the recent experimental investigations of impacting sprays have been conducted in specially constructed test rigs or bombs. To make the analysis of results as simple as possible the "wall" on which the spray impacts is often a flat plate. Both normal and oblique impacts have been studied in this way [3, 4]. Some experiments have also attempted to simulate the effect of swirling flows in engines by incorporating a cross-flowing gas into the rig [5]. However, it is extremely difficult to measure droplet sizes and velocity distributions in the near-wall region. Computational modeling offers a promising alternative for the purpose of obtaining detailed information on spray impingement characteristics. The first experimental scientific investigations into certain aspects of drop impact were conducted by Tomlinson [6, 7], Worthington [8, 9], and Thompson and Newall [10] in the second half of the nineteenth century. At the end of the last century, the first droplet wall interaction model was proposed by Naber and Reitz [11]. In their model, an impinging droplet is assumed to stick on the wall in a spherical form ("Stick" model), reflect elastically ("Reflect" model) or move tangentially along the surface like a jet ("Jet" model). One of the limitations of this model is the conditions for the occurrence of each regime which is not specified in relation to experimental data. Later, Senda et al. [4] developed an impingement model to predict the secondary atomization of the droplets impinging on a wall, the liquid film formation, and the heat transfer between the wall film and the heated wall. This work was mainly based on the experimental investigation on hot walls of Wachters et al. [12] and the predicted results, although they were closer to the experimental results than the ones of previously developed models, were for only one case of injection and impinging conditions. In 1995, Bai et al. [13] proposed a model to predict the outcomes of diesel spray droplets impacting on a wall with temperatures below the fuel boiling point, which has been improved later through the refinement of the quantitative criterion for the regime transitions and the extension of the model to gasoline engine conditions (Bai et al. [14]). The regime boundaries were derived from experimental data and reports collected in the literature. The model solved the conservation of energy equation for an impinging parcel and each incident droplet parcel could produce up to six splashing parcel. The secondary droplet sizes resulting from splash followed characteristic distributions. The model produced satisfactory results for the test case selected by the authors but no clear evidence of general applicability could be inferred from the published results.

The present paper reports a numerical study of a spray impinging on a surface through a crossflow. This work is intended to study the performance of the model of Bai et al. [14] with new regime transition criteria for the representation of the spray impingement phenomena in a three-dimensional configuration. In fact, in addition to the improved transition criteria applied in the present model, also the transition criteria between deposition and splash of Cossali et al. [15], Mundo et al. [16], Senda et al. [17] and Huang et al. [18] have been assessed in the same global model for the configuration of the experimental work of Arcoumanis et al. [19].

The flow configuration is shown schematically in Fig. 1, and consists of a spray stream injected through the upper wall of a rectangular channel. The injector is inclined at 20 ºC (in relation to the vertical plane), in the downstream sense of the channel flow. The cross section of the computational domain is 0.086 × 0.032 m^2, whilst the channel length is 0.350 m. The location of the injection point (Z_{in}) is 0.05 m far from the inlet plane ($Z_{in}/H = 1.563$) and on the symmetry plane.

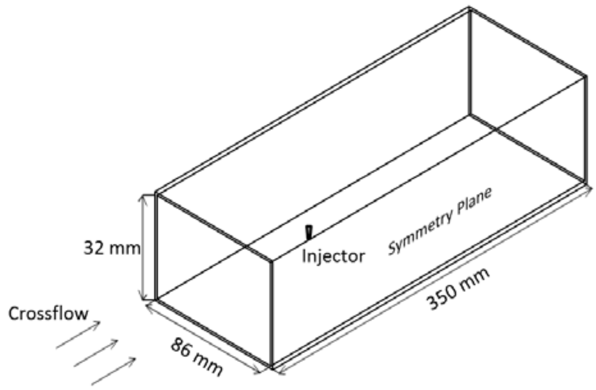

Fig. 1 Schematic diagram of the flow geometry.

After this section, the paper first describes the mathematical model, which includes the transition criteria incorporated into the base model. In the third section, the results obtained with the different correlations are discussed and the final section summarizes the main findings and conclusions of this work.

2. Mathematical Model

The numerical results presented in this paper are based on an Eulerian/Lagrangian approach, which is described in detail in Refs. [20, 21], and only the main features are summarized here.

The fluid phase is treated as a continuum by solving the partial differential equations in a fixed reference frame, which represent each particle and its properties of interest. The turbulence is modeled by mean of the well-known "k-ε" turbulence model, which was found to predict reasonably well the mean flow [22] and the QUICK (quadratic upwind interpolation for convective kinematics) scheme of Leonard [23] is used in order to evaluate the convection terms in the discretization process. The dispersed phase was treated using a Lagrangian reference frame where the particle trajectories were obtained by solving the particle momentum equation through the Eulerian fluid velocity field, and the interaction between the continuous and dispersed phase is introduced by treating particles as sources of mass, momentum and energy to the gaseous phase [24].

The computational domain (Fig. 1) has six boundaries: an inlet and outlet plane, a plane of symmetry and three solid walls at the top, bottom and side of the channel. At the inlet boundary, it is assumed that the crossflow has a constant horizontal velocity component through the entire cross-section while the other two velocity components are set to zero. At the outlet plane, there is a free boundary and no action for transport equation is required. At the symmetry plane, the normal velocity component vanishes as well as the gradients in the normal direction of the other variables. At the three solid surfaces, the normal components of the velocity are set to zero whilst in the other directions wall functionsdescribed by Launder and Spalding [25] are employed for the velocity and turbulence quantities.

Regarding the dispersed phase, it is assumed that the particles are sufficiently dispersed so the interaction between droplets is negligible. In addition, since no reliable atomization model is yet available, an empirical procedure is used to estimate the characteristics of the spray at the exit of the injector. However, due to the limited experimental data available, it is assumed that the droplets are spherical, the spray is dispersed so that the droplet collision/coalescence can be neglected, and the droplet aerodynamic breakup and evaporation are ignored (the measurements were performed at ambient pressure and temperature). Thus, the measured PDF (probability density function), which was taken in particular plane downstream the spray flow, is then reproduced at the exit injector. This method is described in detail in Refs. [13, 20]. The model of Bai et al. [14] considers four impingement regimes: stick, rebound, spread and splash. The existence of these regimes depends on the properties of the impinging droplets and the impingement surface, including whether the latter is dry or wetted [13]. For both dry and wetted wall, the spread-splash regime transition conditions were derived from the Stow and Hadfield [26] data, giving rise to a critical Weber number dependent on the

Laplace number. The regime boundaries between stick/rebound and rebound/spread (derived from Lee et al. [27] data) for wetted walls are set with the critical Weber number of 2 and 20, respectively.

Mundo et al. [16] have investigated multi-droplet impingement on a rough surface and have presented a criterion between the deposition and splash regimes. This empirical correlation is based on the droplet Reynolds and Ohnesorge numbers and has been used in many models since then. Despite the fact that the correlation has been deduced for dry surfaces, it is considered that the wetted wall behaves as a very rough surface. Cossali et al. [15] investigated the same regime transition by analyzing a large number of pictures and found a correlation based on the Weber and Ohnesorge numbers. Later, Senda et al. [17] followed the experimental data of Cossali et al. [15] and found a new criterion which was function of the Laplace number. Recently, experimental observations of droplet impingement with different fluids have been conducted by Huang et al. [18] and a new correlation based on the Weber and Reynolds number has been proposed to predict the deposition-splashing boundary. Table 1 highlights the main characteristics of the base model and the new transition criteria studied.

Deposition is a combination of two physical phenomena, namely "stick" and "spread" in which the arriving droplets are assumed to coalescence to form a local film and no secondary droplets are ejected. The normal component of the droplet kinetic energy prior to the impact is assumed to convert into a dynamics pressure, whereas the original droplet tangential momentum acts towards the increase of the local film tangential momentum. Rebound applies when a droplet bounces against a wetted wall with low impact energy. The air trapped between the bouncing droplet and the liquid film causes low energy loss. To determine the rebound velocity components, the relations for a solid particle on a wetted surface have been used [28].

The base model under study is incorporated in a three-dimensional computational method based on the solution of the Reynolds-averaged Navier-Stokes equation for the gas phase, and a SSF (stochastic separated flow) model based on the eddy lifetime for the particle phase.

3. Results and Discussion

The predictions presented in this section are compared and assessed with experimental data. The main objective of this work is to evaluate the performance of the spray impingement model of Bai et al. [14] with different regime transition criteria for the specific configuration of the experimental work of Arcoumanis et al. [19].

Fig. 2 shows the four different measurement locations where the present results will be compared with the experimental data for the cases of crossflow rates of 5 m/s and 15 m/s. The four different positions a, b, c, and d are located in the center of the wind tunnel and lie respectively at 12, 15, 20, and 25 mm downstream of the injector and within a horizontal plane 5 mm above the impingement wall.

It is assumed that the relative wall film thickness (δ) is the order of unity [4]. To note that the measurements data have size classes of approximately 25 μm while in this study a more precise size classes of 15 μm have been used, which can lead to some discrepancies. In Figs. 3-10, the dashed lines with closed circles correspond to the measurements of Arcoumanis et al. [19], while the solid lines with open symbols correspond to the predicted results: the triangles, the squares, the diamonds, the gradients and the rightward triangles correspond to the transition criteria of Bai et al. [14] (Criterion A), Cossali et al. [15] (Criterion B), Huang et al. [18] (Criterion C), Mundo et al. [16] (Criterion D) and Senda et al. [17] (Criterion E), respectively, which are inserted into the same base model.

Fig. 3 shows the measured and predicted size distributions of droplets moving downward through a crossflow of 5 m/s. Despite the different deposition/splash boundaries evaluated, good concordance is verified between them (only Criterion

Table 1 Impingement regimes and transition criteria.

	Authors	Wall status	Regime transition state	Critical Weber number
Base Model	Bai et al. [14]	Dry	Deposition/Splash	$We_c \approx 2{,}630\ La^{-0.183}$
		Wetted	Stick/Rebound	$We_c \approx 2$
			Rebound/Spread	$We_c \approx 20$
			Spread/Splash	$We_c \approx 1{,}320\ La^{-0.183}$
New transition criteria studied	Cossali et al. [15]	Wetted	Coalescence/Splash	$We_c = (2{,}100 + 5{,}880\ \delta^{1.44})/Oh^{-0.4}$
	Mundo et al. [16]	Wetted	Deposition/Splash	$We_c = 3329.29/Re^{0.5}$
	Senda et al. [17]	Wetted	Deposition/Splash	$We_c = (2{,}164 + 7{,}560\ \delta^{1.78})\ La^{0.2}$
	Huang and Zhang [18]	Wetted	Coalescence/Splash	$We_c = (25 + 7\ \delta^{1.44})^4/Re$

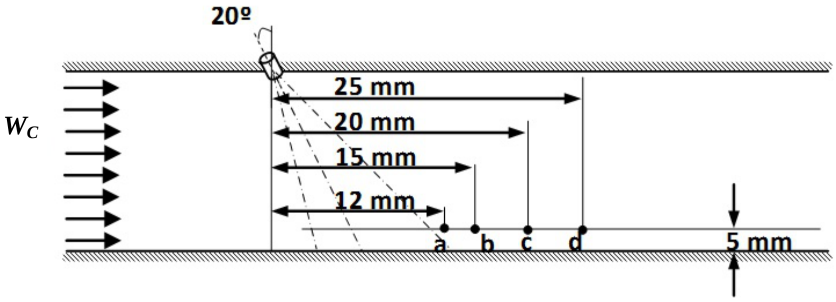

Fig. 2 Illustration of the measurements.

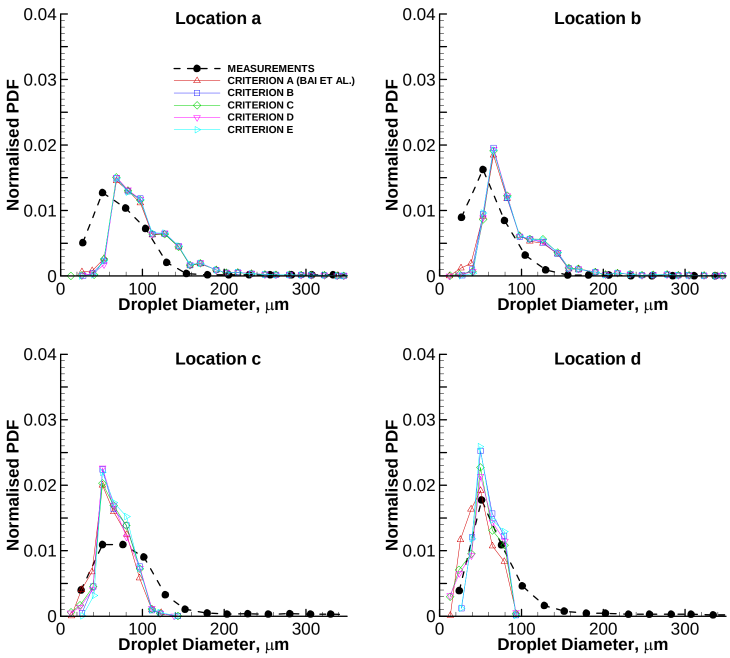

Fig. 3 Size distributions of the downward-moving droplets for a crossflow velocity of 5 m/s.

A shows a slight different behavior for smaller and/or larger droplet diameters at locations c and d) but they still show over-predicted peak values at all the locations considered as well as a rightward shift of the mode of the droplet diameters (or more frequent droplet diameter) at the locations a and b in comparison with the measurements. These discrepancies may be related to the uncertainties with the expected initial characteristics of the spray as well as all the procedures used to estimate those initial conditions (in order to reproduce the spray at the early stage after being generated). In addition, it can be seen at the three locations closer to the injector that the number of smaller droplets is under-estimated, which makes either the increase of the mode value or the over-estimation of the larger droplet diameters. In the specific case of the location c, both smaller and larger droplet diameters are under-estimated, which causes a greater over-estimation of the peak value. Another observation is that at both location c and d, the droplets with diameters larger than 120 μm do not appear in the results contrary to what happens with the measurements.

For the normalized PDF of the upward-moving droplets, the results are presented in Fig. 4 with the presence of a 5 m/s crossflow but in this case the results show very different behaviors. From the figure, it is easily seen that the Criterion E shows difficulty to find upward-moving droplets. This is due to the fact that the critical threshold to reach the splashing regime is in general much higher than in the other correlations, originating fewer secondary droplets and, consequently, altering the corresponding final outcome. In fact, it is seen at location b that one of the point estimated does not appear in the figure because it lies very far from the range limit specified, while at location c the only two size classes observed are far from having a behavior similar to the other correlations. In addition, at location a, no upward moving droplets are found with this correlation and at the location further away from the injector (location d), a distinct distributionis seen. In contrast, the Cossali et al. [15] case (Criterion B) presents numerical predictions that lie quite close to the measurements, despite still slightly over-predicting the droplet diameter peak value and under-estimating the droplets with a diameter of about 100 μm. For the other three cases, the peak-values are over-predicted and shifted to the left—in particular the Criterions C and D. The larger droplets found in the simulation are under-estimated, which may be one cause for the over-estimation of the most frequent droplet diameters.

In relation to the velocity-size correlations for droplets moving downward and upward at the four locations considered with the presence of a 5 m/s crossflow, the results are presented in Figs. 5 and 6. In the case of the droplets moving towards the wall, it is clear that further improvement must be done in order to minimize the difference between predicted and measured results. In general, the velocity profiles are under-estimated for the entire range of droplet diameters,

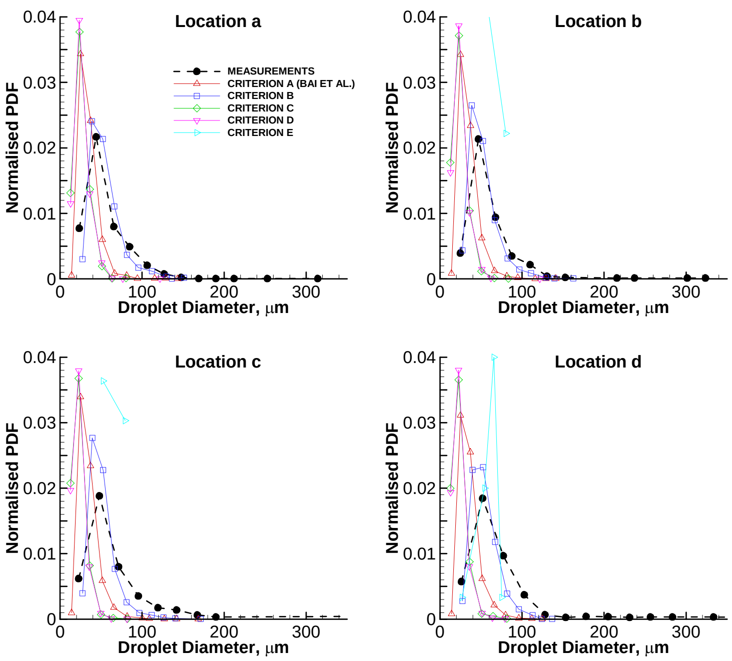

Fig. 4 Size distributions of the upward-moving droplets for a crossflow velocity of 5 m/s.

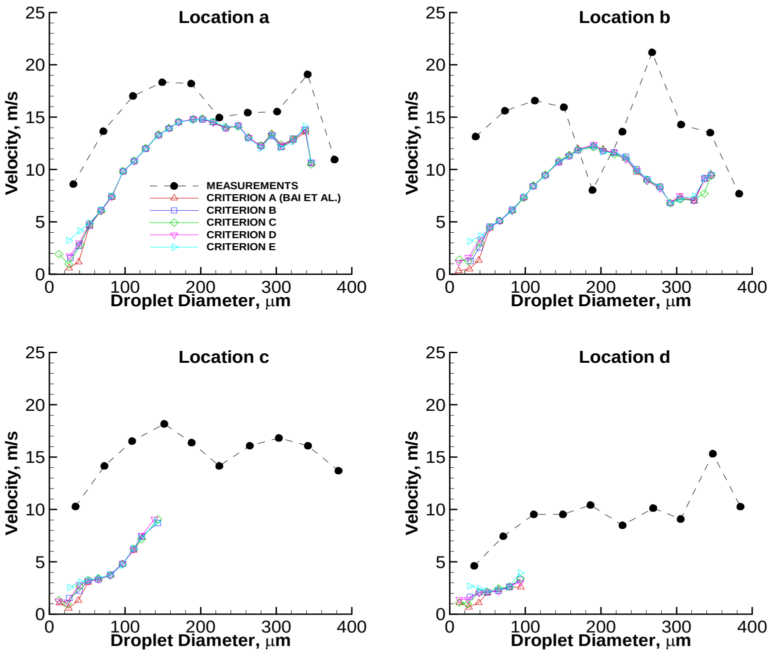

Fig. 5 Velocity-size correlations of the downward-moving droplets for a crossflow velocity of 5 m/s.

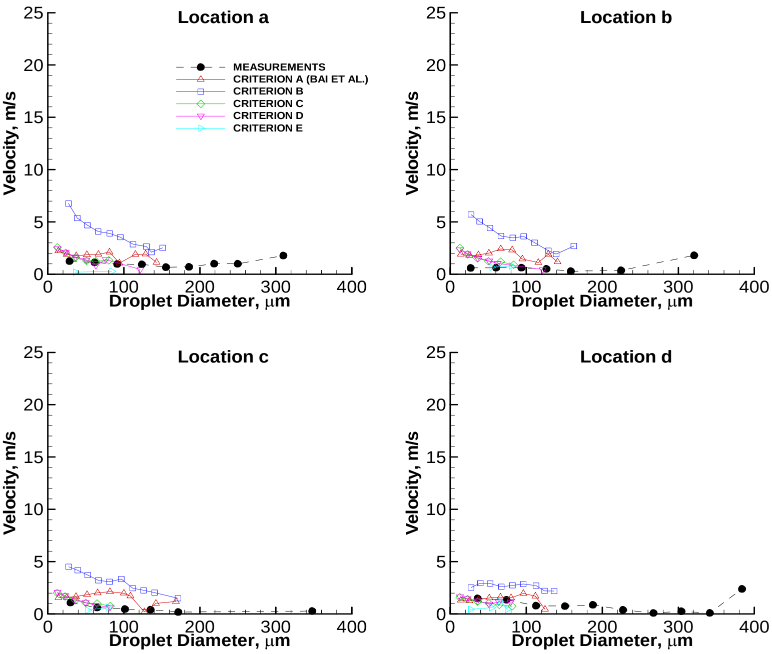

Fig. 6 Velocity-size correlations of the upward-moving droplets for a crossflow velocity of 5 m/s.

except at the location b where there is a slight range (droplets with diameter around 200 μm) in which the predicted velocity is over-estimated in relation to the measurements. In addition, even the main behavior of the velocity profile is different: at locations c and d, it is seen that the larger the droplet diameter, the greater the upward velocity, whereas in the case of the experimental data the behavior is not so straightforward. To note also that there are not found droplet size classes as large as those found in the measurements. In fact, this particular matter is more evident at locations c and d where the measured maximum size classes are, respectively, around 2.7 and 4 times greater than the estimated ones. On the other hand, good agreement is verified between all the different regime transition thresholds evaluated at the four locations. Fig. 6 presents the upward moving droplets and reveals the difficulty of modeling the droplets resulting from rebound and splash regimes, which definitively calls for an improvement of this particular matter. The maximum size class found never exceeds 180 µm, whereas in the measured case they can extend until almost 400 µm. In addition, it can be seen that the Criterion B result is somewhat overestimated. This may be due to the fact that the critical threshold is inversely proportional to the droplet diameter, which makes that only the larger droplets and thus a lower threshold can reach the splash regime. This fact leads to a slight increase in the splash kinetic energy and, consequently, a slight increase in the upward velocity. This combination between larger secondary droplets with greater velocity may be one of reason for the difference in the upward moving droplets results.

Directing attention to the crossflow rate of 15 m/s, the measured and predicted size distributions of droplets moving downward and upward are presented in Figs. 7 and 8, respectively. Fig. 7 reveals great consistency between the correlations considered but it still over-predicts the most frequent droplet diameter at all the locations, and also present a rightward shift of the mode of the droplets diameters at locations c and d and a leftward shift at location b. At locations a, c and d, there is an under-estimation of the droplets with smaller diameters, which is balanced with the over-prediction and the rightward shift of the peak value. In the upward-moving case, as in the simulation made for a crossflow rate of 5 m/s, the results show very specific behaviors dependent on the correlation used. All have a leftward shift at all the location, except Criterion B at location d. In fact, this case is the one which is more similar to the measurements. The Criterions C and D present a more noticeable over-predicted mode of the droplet diameters at all the locations, while in the Bai et al. [14] case this behavior is only found at location d. Just as with the results presented with a crossflow of 5 m/s, the correlation proposed in Senda et al. [17] does not present satisfactory results possibly due to the reason presented above.

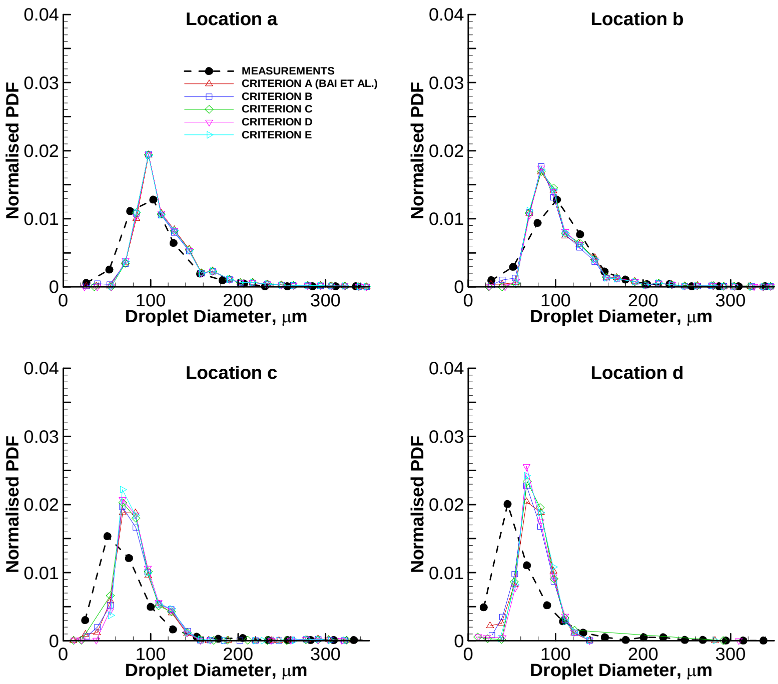

Fig. 7 Size distributions of the downward-moving droplets for a crossflow velocity of 15 m/s.

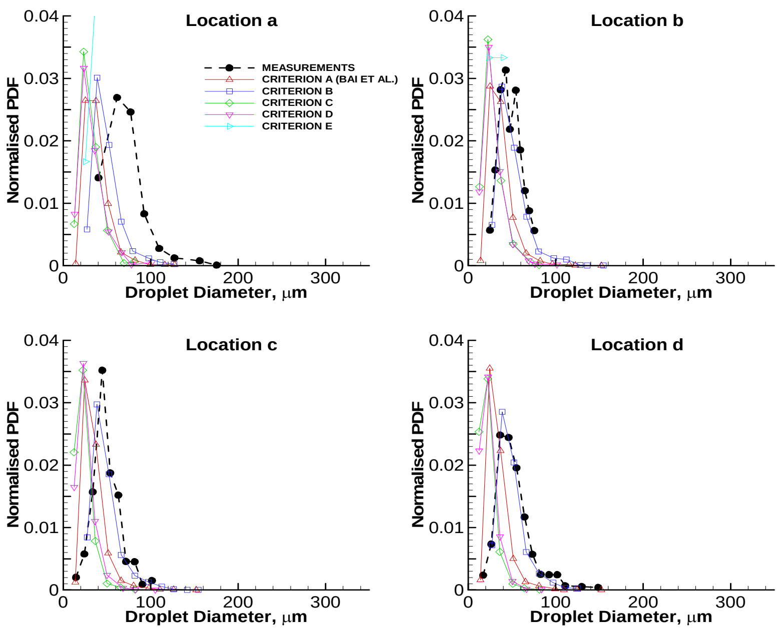

Fig. 8 Size distributions of the upward-moving droplets for a crossflow velocity of 15 m/s.

Figs. 9 and 10 depict the velocity-size correlations for droplets moving downward and upward, respectively. In the first case, the different transition criteria evidence good consistency between them but not with the measurements. In fact, the velocities verified are under-estimated at all the locations and along the entire diameter range. To note also that the maximum size class estimated is still lower than the measured as seen in the results for a crossflow of 5 m/s. Fig. 10 presents the upward-moving droplets and illustrates some discrepancies between the predictions and the measurements as stated also in Fig. 6 in the lower crossflow rate simulation.

4. Conclusion and Future Work

In conclusion, and comparing the five transition criteria studied, as it would be expected the results of the downward moving droplets show good concordance between them (principally at the locations closer to the injector plane) since the majority of the parcels comes directly from the injector and impinge on the solid wall and, consequently, the post-impingement characteristics under the splash regime do not have much influence. This situation reinforces the influence of the initial conditions on the outcome and, consequently, the necessity of an accurate atomization model to determine the characteristics of the spray in the near-nozzle region. On the other hand, the upward moving droplets are due either to rebounding or disintegration of the incident drops. In the specific case of the PDF graph of the upward moving droplets, the results obtained with the correlation of Cossali et al. [15] reveals a better agreement with the measurements than the other ones evaluated. However, in the case of the velocity-size plot, the opposite is verified: the transition criterion of Cossali et al. [15] deviates from the results obtained with the other thresholds and, in particular, deviates from the measurements.

The results presented in the previous section revealed a certain difficulty to reproduce correctly the upward moving droplets. This situation may be related to the limitation of the model in relation to the transport of the liquid film deposited on the solid wall. Despite the base model considers up to six parcels resulting from the splash of the incident drops, it does not effectively take into account the thickness of the liquid film in the secondary droplet characteristics as well as its possible movement with both the impact of incident drops and the presence of the crossflow.

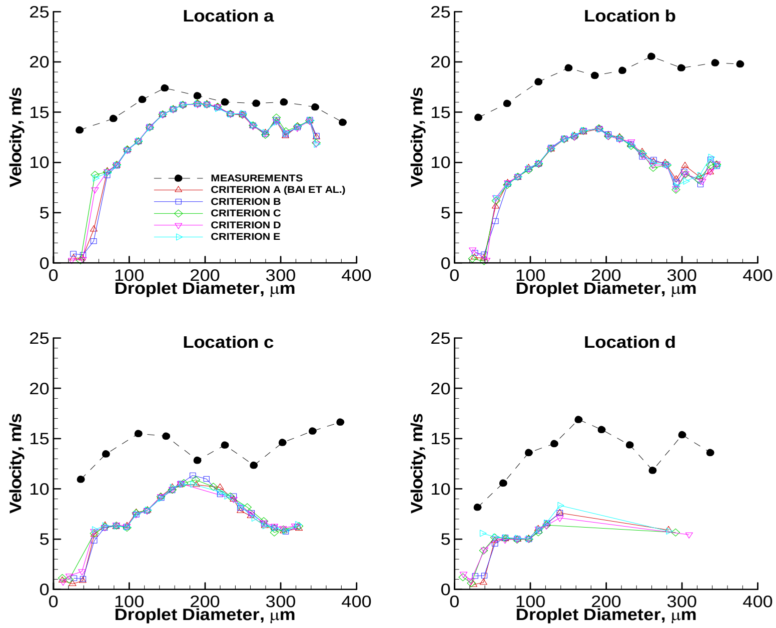

Fig. 9 Velocity-size correlations of the downward-moving droplets for a crossflow velocity of 15 m/s.

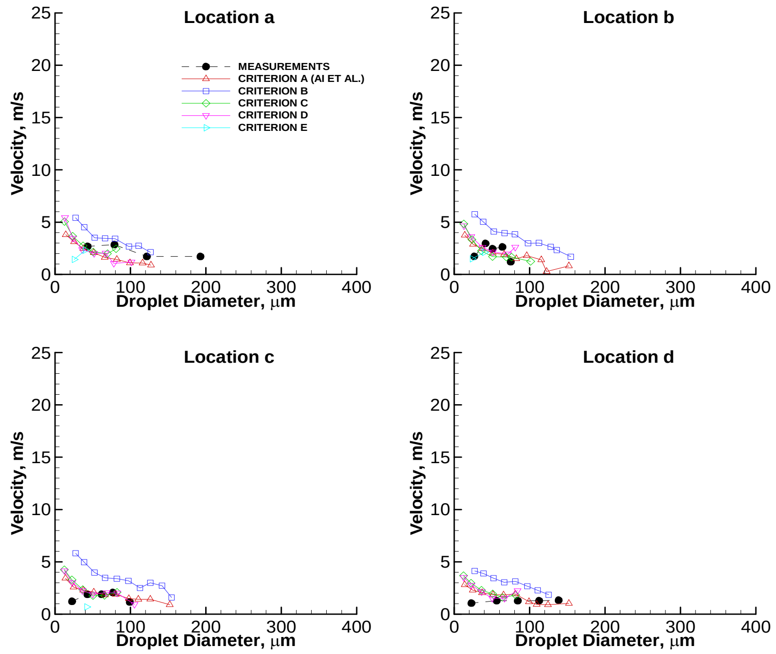

Fig. 10 Velocity-size correlations of the upward-moving droplets for a crossflow velocity of 15 m/s.

Another aspect that calls for further research is related to the refinement of the secondary droplets characteristics in order to improve the quality of the outcomes. Thus, attention must be given to the dissipative energy loss, which is a fundamental parameter to estimate the post-impingement characteristics (specifically to evaluate the velocity of the secondary droplets) in the splash regime and, consequently, to model adequately the spray impingement process.

Acknowledgments

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