An Evaluation of Atomization Models for Dense Sprays

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Abstract
Calculations of a transient atomization process are presented, which simulates fuel injection of sprays in gasoline direct injection engines. Only non-reacting sprays are considered with the focus on the atomization process. The FIRE code, developed by AVL, is used as the platform to test three different atomization models: (i) Taylor Analogy Breakup (TAB) model; (ii) surface wave instability (WAVE) model; and the more recent (iii) FIPA (Fractionnement Induit Par Acceleration) model. Comparisons of calculations with experimental data reveal significant discrepancies regardless of the atomization model used. It is acknowledged that, in this study, only the standard model constants are adopted and that may be further optimised to improve the calculations. However, the fact remains that all the atomization models start with an initial distribution of spherical droplets at the injector tip. An assumption that is not supported by recent measurements which show that fluid elements rather than spherical droplets dominate this early zone.

1. Introduction

Modelling of fuel spray combustion is a highly complex process, which involves the phenomena of the disintegration of fuel sheets and ligaments into droplets which are poorly understood. Breakup and atomization in the formation of dense sprays is a typical example of such processes where semi-empirical models are used and where there is a severe shortage of relevant and reliable data. This near nozzle region of the spray is obviously critical as it determines the nature of the droplet evaporation, coalescence and combustion processes, which take place further downstream in the fully developed spray. There are a number of excellent reviews and monographs on sprays, [1-2] which highlight the lack of understanding, the crude modelling of the atomization process and the need for improvements. There are a number of models for spray breakup and atomization described in the literature and some of these are implemented in commercial codes used by the spray community, particularly in the automotive industry [3-5]. There are also significant efforts made by various groups to generate new data for dense spray atomization and to enhance the current models and validate them against these data [6-8]. Most of the models used in commercial codes make the assumption that atomization involves the break up of large spherical droplets into smaller ones [9]. None of these models have yet been adopted

successfully the common experimental observation that liquid filaments dominate the early region of sprays long before spherical droplets are formed.
This paper forms an initial attempt to address the important issues of spray atomization by comparing current numerical capabilities with experimental measurements. The FIRE code, developed by AVL, is used as a numerical platform with a standard *k-e* model for turbulence. The modelled experimental configuration consists of a pressure swirl injector operating at 5 MPa and forming a hollow cone of spray which issues into stagnant air at atmospheric pressure and ambient temperature. The spray injection duration was 1.16 ms, with a delay of 0.36 ms between the needle opening and the appearance of fuel form the nozzle tip. In this paper, three breakup models have been examined and the model predictions have been evaluated against experimental data reported by Wigley et al. [10,11]. Spatially-resolved measurements of two component velocity and droplet size distribution at various planes across the spray cone have been made using Phase Doppler Anemometry (PDA). The data represent the complete time history during the injection and spray development process and cover the physical domain from the injector tip to 50 mm downstream.

2. Numerical Issues

The numerical study was performed using the AVL-FIRE version 7.3 [12]. The governing equations for conservation of mass, momentum and energy were solved for the three-dimensional two-phase flow. The transient spray simulation was based on the Eulerian-Lagrangian method. In this method, only the carrier (gas) phase is treated as a continuum, subject to the equations of continuum fluid mechanics. The dispersed (liquid) phase is treated as if it were composed of particles. Turbulence was implemented using the *k-e* model. Dukowicz [13] assumed uniform droplet temperature that received energy conducted from uniform properties surrounding gas. This, either heats the droplet, or provides the evaporation energy. A statistical coalescence model was used to determine the collision probability between the droplets in the same computational cell, according to O'Rourke and Bracco [14].

2.1 Atomization models

O'Rourke and Amsden [15] developed a droplet break-up model called the "TAB" (Taylor Analogy Breakup) model, which is based on Taylor's (1963) analogy between an oscillating and distorting drop and a spring-mass system. The external force acting on the mass, the restoring force of the spring and the damping force are analogous to the gas aerodynamic force, the liquid surface tension force, and the liquid viscosity force, respectively. This leads to the following equation:-

$$\ddot{y} = \frac{2}{3}\frac{r_g U^2}{r_l r^2} - \frac{8s}{r_l r^3} y - \frac{5m_l}{r_l r^2}\dot{y} \qquad (1)$$

where y is the normalized droplet distortion. The model predicts that break up occurs if and only if $y > 1$. U is the relative velocity between the gas and the droplet, r is the droplet radius, r_g and r_l is the gas and the liquid densities respectively and s is the liquid surface tension.
Droplet break up in the WAVE model [16] is due to the unstable growth on a liquid surface of waves, subjected to an infinitesimal axi-symmetric displacement. The maximum growth rate, *?* , and its corresponding wavelength, L, are related to the pertinent properties of the liquid and gas by:-

$$\frac{\Lambda}{a} = 9.02\frac{\left(1+0.45Z^{0.5}\right)\left(1+0.4T^{0.7}\right)}{\left(1+0.87We_g^{01.67}\right)^{0.6}} \tag{2}$$

$$\Omega\left[\frac{r_l a^3}{s}\right] = \frac{0.34+0.38We_g^{1.5}}{(1+Z)\left(1+1.4T^{0.6}\right)} \tag{3}$$

where
$$T = ZWe_g^{0.5} \tag{4}$$

We_g is the gas Weber number ($We_g = r_l U^2 r/s$), and Z is the Ohnesorge number ($Z = We_l^{0.5}/Re_l$); which represents the ratio between the droplet Weber number ($We_l = r_g U^2 r/s$) and the Reynolds number ($Re_l = 2rgUr/m_g$). Where r is equal to, in this case, a, which refers to the radius of the parent liquid droplet. The break up time calculated from the relationship (t_{bu} = B3.726a/$\Lambda\Omega$). Where is B a constant equal to 1.73. Liquid break up is modelled by postulating that new drops of radius, r, are formed from the bulk liquid or "blobs", with a characteristic radius a, with

$$r = 0.6\Lambda\,, \quad (\Lambda \leq 1.67a) \tag{5}$$

or
$$r = \min\left\{\left(3pa^2U/2\Omega\right)^{0.33}, \left(3a^2\Lambda/4\right)^{0.33}\right\} \quad \text{for } (\Lambda > 1.67a) \tag{6}$$

Baritaud et al. [17] proposed a hybrid approach to model the high-pressure spray dynamics. Using the WAVE model in the atomization zone and the FIPA model, which differentiates between the drop break up modes as dependent on its Weber number We_l. This is based on Pilch's experimental correlations, which give different characteristic breakup times (t_{ch}) as the following:-

Vibrational break-up
$$t_{ch} = 6\left(2We_l - 12\right)^{-0.25}; 12 \leq 2We_l \leq 18$$

Bag break-up
$$t_{ch} = 2.45\left(2We_l - 12\right)^{-0.25}; 18 < 2We_l \leq 45$$

Bag-stamen break-up
$$t_{ch} = 14.1\left(2We_l - 12\right)^{-0.25}; 45 < 2We_l \leq 350 \tag{7}$$

Sheet stripping
$$t_{ch} = 0.766\left(2We_l - 12\right)^{-0.25}; 350 < 2We_l \leq 2670$$

Wave crest stripping
$$t_{ch} = 5.5; 2670 \leq 2We_l$$

While the breakup time t_{bu} is calculated by:-

$$t_{bu} = Ct_{ch}\left(\frac{r_l}{r_g}\right)^{0.5}\left(\frac{2r}{U}\right) \tag{8}$$

C is a constant analogous to the constant B in the WAVE model. In general all three breakup models have critical Weber numbers We_l^* equal to 6.

2.2 Boundary conditions

A schematic of the pressure swirl nozzle used by Wigley et al. [10,11] is shown in Figure 1. It has an exit diameter of 0.9 mm and swirl vanes upstream from the exit plane through which liquid fuel is injected to assist in the formation of droplets. A cross section of the three-dimensional computational domain used here is shown in Figure 2. It consists of hexahedron mesh with the injector centred at its top where symmetry conditions are

assumed. Outlet boundaries are specified at the walls and the base. The computational domain has an unstructured mesh size of 100 x 110 x 100 mm.

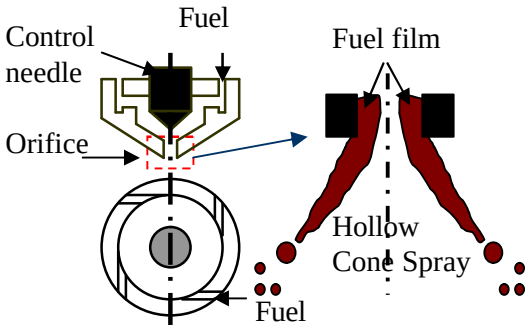

Fig. 1 Schematic of hollow cone spray formation

A Rossin-Ramler droplet size distribution, shown in figure 3, was adopted at the exit plane of the injector with the following parameters: q = 15, X = 150. The maximum droplet diameter specified at the nozzle exit plane was 180 micron. This was obtained from the maximum dimension of the swirling liquid annulus upstream of the exit plane of the injector [18]. Fuel injection occurs over a period of 1.16 ms. The liquid injection velocity and the spray cone half angle for the injection occurs are shown, versus injection time, in Figures 4a and 4b, respectively. These conditions are a very close match to those used experimentally.

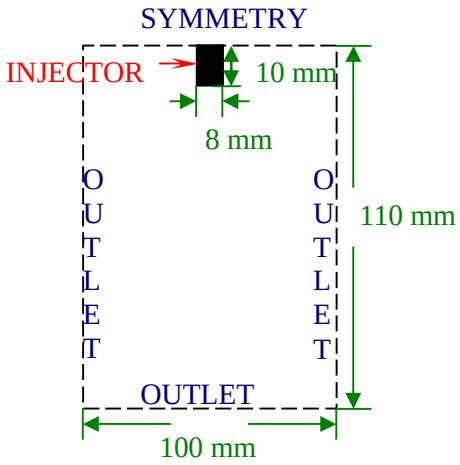

Fig. 2 Computational domain with Boundary Conditions

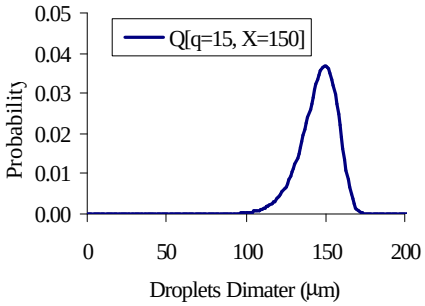

Fig. 3 Rosin-Ramler droplet diameter distribution at injector exit plane

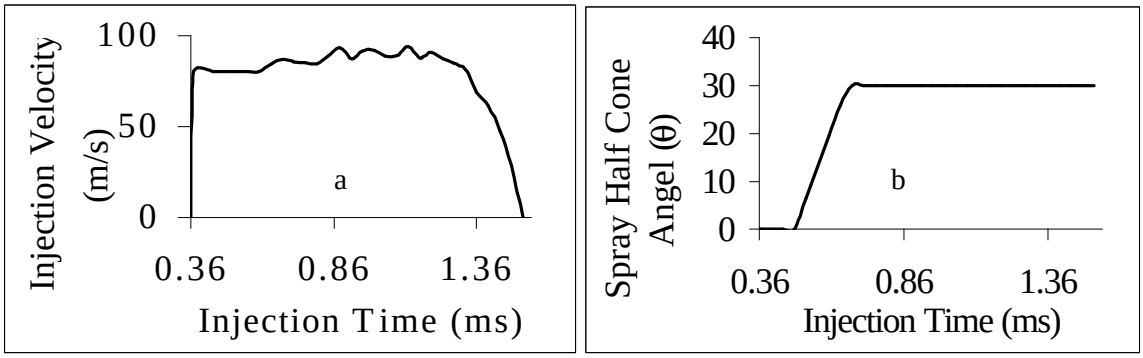

Fig. 4 Initial conditions, a) Spray Half Cone Angle θ, b) Injection Velocity Profile

3. Results and Discussion

To evaluate the evolution of the spray field from injection to discharge, spray patterns computed using the three atomization models are to be shown, at various times, for the spray and chamber symmetry plane. Two-dimensional slices of the spray patterns are presented in figure 5 for the times of t = 0.72, 1.12, 1.52 and 1.92 ms after the start of injection. Computations using the TAB, WAVE and FIPA models, from left to right, are shown side by side. The plots are colour coded with respect to droplet size with red referring to the largest droplets, 180micron, and dark blue referring to smallest droplets, 1micron.

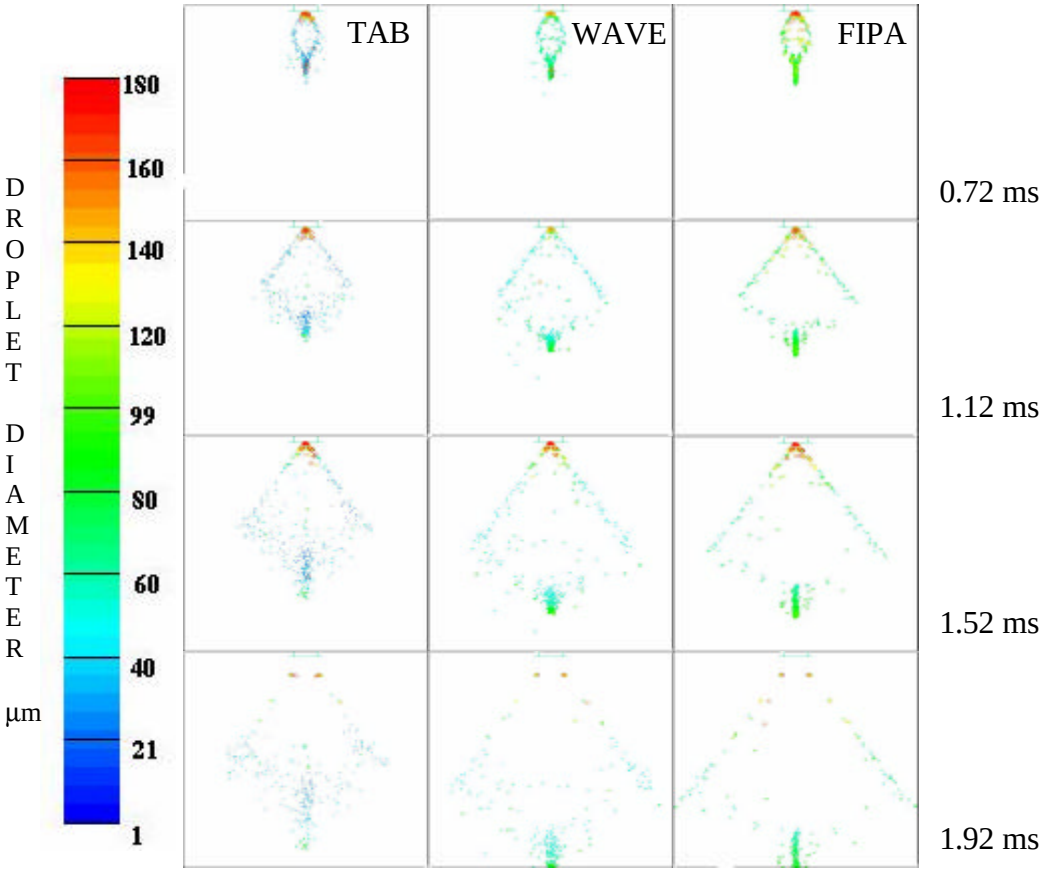

Fig. 5 Planar spray patterns of the droplet size distribution for the three computational models

These images reveal, not only the time history of the spray atomization and droplet distribution rates during the spray cone development, but clearly highlight the differences between the various modelling approaches. At t=0.72ms, most of the spray is still jetting straight down the spray axis due to the fact that, for the first 0.15ms of injection, the half cone angle, θ, is zero, see figure 4b. By the end of the injection process, t = 1.52 ms, all three atomization models show that the expected half cone angle of 30 degrees is already fully established. The TAB model shows the spray with the slowest penetration while the FIPA model yields the fastest. It is clear from the plots at t = 1.52 ms that the droplet diffusion to the inner core of the jet has the largest population for the TAB model while the FIPA model gives an almost distinct hollow cone. At t=1.92, the injection of fuel through the nozzle is complete and the existing downstream droplets start to slow and tend to stabilise.

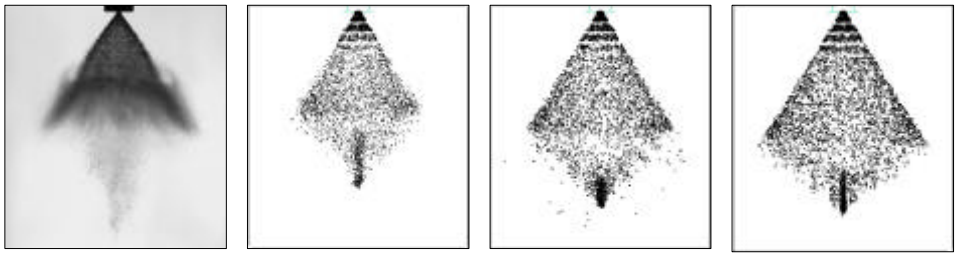

Fig. 6 Comparison between the experimental spray pattern and the predictions spray patterns after 1.52 ms from the injection

A comparison between an experimental CCD image, frame size 70 x 60 mm, of the spray and the computed spray patterns at t = 1.52 ms after the start of injection, is shown in figure 6. These images are not planar resolved but include the entire spray droplet field within the chamber. It is noted that the qualitative features of the spray envelopes are adequately reproduced by the three models. However, an interesting feature of the imaged spray that is not reproduced numerically is the recirculating vortex, starting at 30mm from the nozzle. This is formed on the periphery of the spray cone due to a shear layer, generated by the slip velocities between the spray and the surrounding environment.

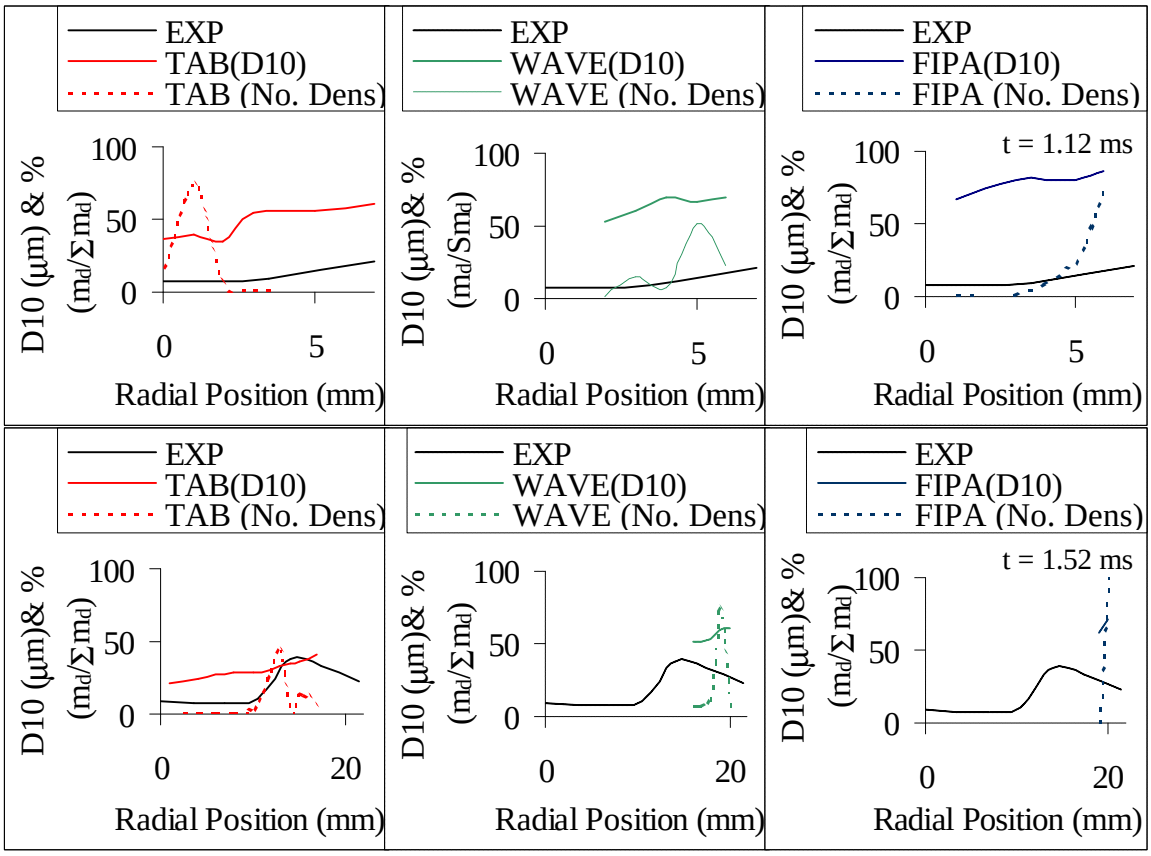

Fig. 7 Predictions of TAB, WAVE & FIPA for the mean droplet diameter (D_{10}) and number density vs. droplet radial position at y = 35 mm at t = 1.12 & 1.52 ms.

On a more quantitative basis radial profiles of the mean droplet diameter, (D_{10}), and droplet number densities computed at y = 35mm from the nozzle tip at times, t = 1.12, and 1.52 ms, after the start of injection, are shown in Figure 7. Computations using the TAB, WAVE and FIPA models are shown side by side.

The measured and computed radial profiles of the mean axial and radial velocities in the symmetry plane of the chamber at 35mm from the nozzle tip and 1.52ms after the start of the injection are shown in figure 8. It is clear, the TAB model produces a droplet distribution covering the entire width of the spray. The WAVE and FIPA models demonstrate that there is a concentration of droplets in the outer radial locations commensurate with the spray angle of the injector. The computed velocity fields with the WAVE and FIPA models show slightly higher velocities on the outer edges of the jet. The atomization process can be inferred from figure 9 which shows the evolution of the mean droplet diameter (D_{10}) versus time for two locations within the chamber, y1 =5 mm and 30 degrees, y2 = 35 mm and 30 degree. Two plots are shown side by side for each of the atomization models. These plots show how the particle diameter changes due to atomization as the fluid travels across the chamber. Atomization is most effective for the TAB model. At t =1.52 ms, the maximum droplet size produced by the TAB model, 35 mm downstream of the injector, is 40 microns while the corresponding maximum for the WAVE and FIPA models are 55 and 60 microns, respectively.

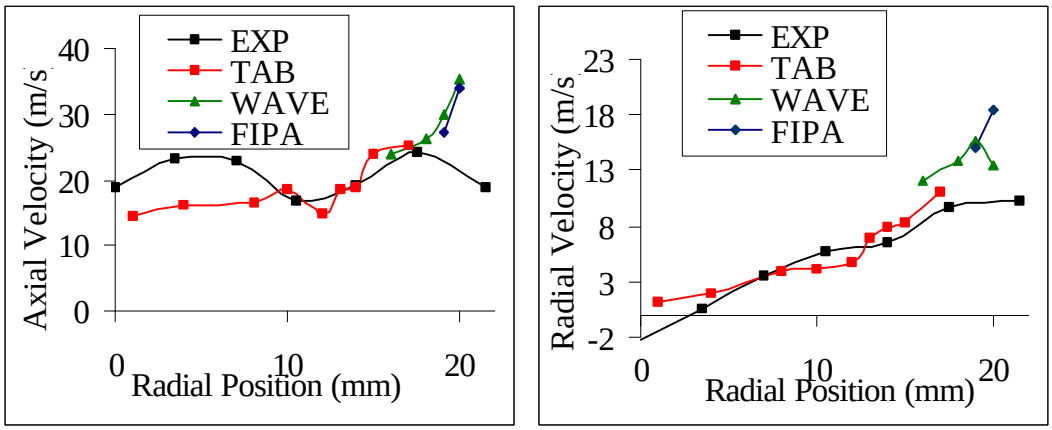

Fig. 8 Mean axial and radial droplet velocity vs. radial position at y = 35 mm from the nozzle tip at t = 1.52 ms

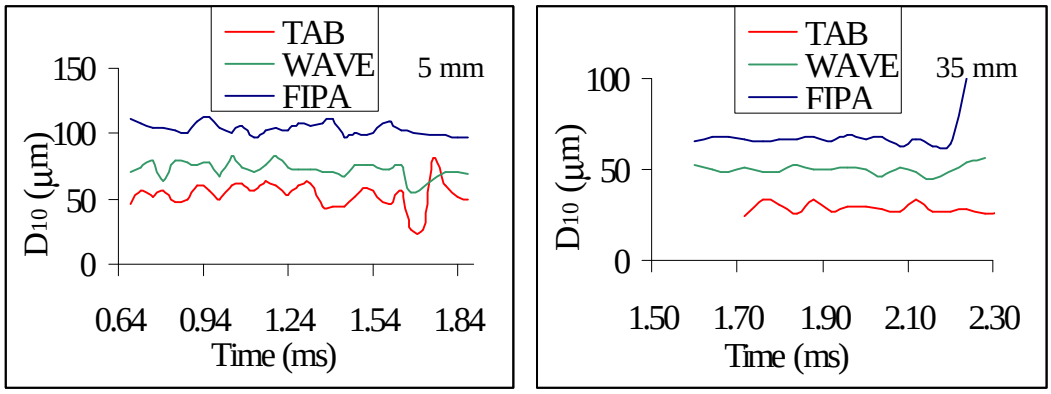

Fig. 9 Predictions of TAB, WAVE & FIPA for the mean droplet Diameter (D_{10}) vs. time at y(1) = 5 mm and y(2) = 35 mm, from the nozzle tip, at θ = 30°.

4. Conclusions

Three atomization models were tested and validated against experimental data collected in the dense spray produced by a pressure swirl atomiser. The FIRE code was used to solve the transient, three dimensional Reynolds Averaged Navier Stokes Equations. Although the initial droplet distribution of spray was assumed, all three models produced a spray pattern

that is qualitatively, rather than quantitatively, similar to the experiments. An assumption had to be made about the initial droplet distribution. Further development of the atomization models is required if quantitatively accurate predictions are required.

5. Acknowledgement

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