Investigation of Thermodynamics Properties Effects on Spray Tip Penetration

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***Abstract*—Different breakup models are applied to numerically model a single-hole n-Hexadecane injector, in order to find the most appropriate model for predicting the spray behavior. The simulations are performed in OpenFOAM by use of dieselFoam solver. Spray tip penetration is calculated by applying the ETAB, Wave and KHRT breakup models. Results show that ETAB breakup model has better agreement with the experimental results, obtained by HP/HT spray rig of Chalmers University of Technology. As turbulence has an important impact on the droplet collision outcomes, standard k-ε turbulence model and two modified versions of this model are applied to the code in order to calculate the spray tip penetration. It is noticed that these modifications make the results approach to the experimental results. By choosing the most convenient model, the effect of ambient pressure and injection pressure are investigated. Increase in the injection pressure leads to an increase in the penetration length, while increase in ambient pressure shows a reverse effect**.

***Keywords*—**Breakup, Droplet Collision, Penetration Length, Pressure and Spray

I. INTRODUCTION

Spray studies, including droplet collision and breakup modeling, have been always of great importance among scientists and engineers because of their vast industrial applications, like painting, spray cooling, injection process in internal combustion engines and furnaces, rain formation, etc. Spray behavior, including the atomization and breakup of droplets during injection process into an internal combustion engines, has close relationship with the performance and efficiency of the engine and hence, the pollutant emissions and fuel consumption control (Kim et al., 2010 and Moreira et al., 2010). A homogenous mixture causes the emission of particle matter (PM) to reduce and improves the combustion efficiency of the engine (Park et al., 2009). Therefore, more accurate understanding of droplet collision and breakup phenomena is of great importance. Droplet collision has been proved to be very difficult to study and model (Park et al., 2009). Restriction of experimental methods in predicting the abrupt behavior of a droplet after collision, measuring range of droplets diameter and defining the satellite droplets properties, makes experimental methods difficult to implement and produce unreliable results (Schmidt and Rutland, 2001). That is why great deals of attention are currently more dedicated to the numerical methods. However, investigating the spray behavior through numerical models is itself very difficult because of limited computational sources and yet-unknown complex concept of droplet collision. Over the years, many numerical models for spray simulation have been developed and the effect of different injection parameters, such as injector geometry, injection characteristics and the ambient properties, on the spray behavior investigated through these models. A complete overview of works done in this field is presented by Moreira et al. (Moreira et al., 2010).

In this work, a single-hole n-hexadecane injector is modeled with different breakup and turbulent models in order to find the most acceptable model for further simulations. Then, by use of the obtained model, the injection properties in different ambient and injection pressures are investigated. In order to verify the accuracy of the results, the obtained numerical results are compared with the experimental results performed at Chalmers University of Technology (Kösters and Karlsson, 2011). The main concern of the current work is focused on best predicting the spray tip penetration. Spray tip penetration is defined as the maximum reachable distance from the nozzle exit. Optimal design of injection conditions is very important to achieve an appropriate penetration length. An over penetration of spray can result in fuel impingement on the combustion chamber walls and an inadequate one can lead to an unsatisfactory fuel–air mixture and consequently reduces the combustion efficiency (Park et al., 2009).

Lots of work on spray tip penetration can be found in the literatures which deal with investigating the effective parameters on penetration length of a spray, optimizing the combustion conditions to reach the optimum penetration length and deriving theoretical and impractical governing correlations. Hiroyasu et al. (1990) and Desantes et al. (2006) showed that the relative magnitude of two opposing forces, namely the kinetic energy of the initial liquid jet and the aerodynamic resistance of the surrounding gas, influenced the penetration length of a spray. Kawano et al. (2004) declared that increase in initial injected fuel temperature yielded the reduction in penetration length of the spray due to

evaporation of the fuel with low boiling point. Lefebvre (1989) determined the best corresponding spray tip penetration to the size and geometry of the combustion chamber in a way that optimized the engine performance.

II. NUMERICAL MODELS

Several sub-models, such as heat transfer, evaporation, breakup, droplet collision, droplet drag and turbulence, should be employed for simulating the spray process. A brief description of some of these models will be presented in the following sections. Detailed information can be found in the addressed references.

A. Breakup Models

In order to accurately model the breakup mechanism due to the liquid-gas droplets interaction, a robust three-dimensional formulation of instabilities is needed. These instabilities occur at the contact surface of two phases and usually resulted from either Rayleigh-Taylor (RT) (Bellman and Pennington, 1954) or Kelvin-Helmholtz (KH) (Reitz and Bracco, 1986) instabilities. The first is caused by the inertia of the denser fluid when the system experiences an acceleration perpendicular to the interface in direction of the denser fluid; the second is a consequence of the viscous forces due to the relative tangential motion of the two phases at the phase-dividing interface (Taylor, 1963).

The breakup of the fuel droplets is determined by using the breakup criterion of the standard TAB model but with a different strategy for the determination of the product droplet size distribution.

1) TAB Breakup Model

The TAB breakup model is based on Taylor's analogy between an oscillating distorting drop and a spring-mass system (Taylor, 1963), where the aerodynamic droplet-gas interaction corresponds to the force term, the damping is due to the liquid viscosity and surface tension plays the role of the restoring force. The radii of the product droplets are determined by an energy balance between the parent and product droplets which, generally, leads to the underestimation of the drop sizes in diesel engine environments. In this model, the necessary condition for drop breakup is reached when

$We > We_{critical}=6$.

Notice that the TAB model is the simplest linear equation which describes a droplet deformation under a forcing, restoring and damping conditions. There is no symmetry assumptions about the deformed droplet in this model, hence, this model can be used to describe lenticular shaped droplet deformations (Taylor, 1963) as observed in experiments by (Liu et al., 1993 and Hwang et al., 1996). A detailed analysis of this model, together with a discussion of its numerical implementation, is given in (O'Rourke and Amsden, 1987 and Amsden et al. 1989).

2) Enhanced TAB (ETAB) Breakup Model

The Enhanced TAB (ETAB) model utilizes the droplet deformation dynamics used in the standard TAB model with a new strategy for the description of the droplet breakup process. In this model, the rate of product drop creation is assumed proportional to the number of the product droplets, with the proportionality constant dependent on the breakup regime. In addition, an energy balance consideration between the parent and product droplets yields an expression for the product droplet velocity component which is normal to their trajectory. Detailed explanation of this model is presented in (Tanner, 1997).

3) Wave Breakup Model

The Wave breakup model (Reitz and Diwakar, 1987) is based on the growth of KH instabilities on the liquid surface at the interface of two phases which have different densities. The result is a general dispersion equation which relates the growth rate of an initial surface perturbation to its wavelength.

In contrast to the ETAB model, the Wave breakup model has no radial velocity component given to the product droplets after drop breakup. Therefore, it is necessary for the user to accurately adjust the initial spray cone angle with respect to the gas density (Kaario et al., 2002).

4) Hybrid Breakup Model of KHRT

Hybrid models combining the droplet breakup model with the wave instability models, in which the primary breakup process is model by Kelvin-Helmholtz (KH) instability (i.e. Wave model) and the secondary breakup process is calculated by use of the Rayleigh-Taylor (RT) approach (Bellman and Pennington, 1954) which reflected the atomization characteristics by the RT instabilities. A comprehensive description of this model can be found in (Beale and Reitz, 1999).

B. Turbulence Models

The most widely used approach for simulating the turbulence is the Reynolds-averaged Navier-Stokes (RANS) equations application. The computational costs of this procedure are acceptable, and the accuracy of the results is adequate for most purposes. K-ε turbulence model (Kösters and Karlsson, 2011) is generally known to yield reasonably realistic predictions of major mean-flow features in most situations (Nishida et al., 2009). Hence in this work, the standard k-ε and two of its modified versions are applied to the simulations. The model constants which are used in these models are listed in Table 1. The description of each symbol can be found in (Kösters and Karlsson, 2011).

Table 1: Constants of different k-ε turbulent models used in the current work simulation

Turbulence model	C1	C2	C3	C_μ	σ_ε	σ_k
Standard k-ε model	1.44	1.92	-0.33	0.09	1.3	1
Tuned k-ε model [10]	1.55	1.92	-0.33	0.09	1.58	1

III. NUMERICAL SOLUTION PROCEDURE

OpenFOAM-1.5 (Open Field Operation and Manipulation) is open-source code which is used here for simulating the spray behavior. The solver used for implementations is dieselFoam. The finite volume method is used to solve numerically the Navier-Stokes equations for any 3D grid of unstructured polyhedral cells.

The geometry under consideration is a 20×20×110 mm rectangular cube with a mesh grid size of 1 mm. The mesh size is the same in all directions and kept unchanged in all of the simulations. N-Hexadecane is used as the fuel injected by the pressure of 600bar into a quiescent ambient of 683 K and 50 bar. A single-hole injector of diameter 140μm and cone angle of 15° is modeled in a common rail injection system with the injection mass flow rate given in Figure 1. The computation time step is set to 1μs and 12000 parcels are injected in each computational cycle. The injection pressures of 100 and 400 bar and ambient pressures of 30, 70 and 90bar are also modeled on order to investigate the effect of pressure on the spray tip penetration.

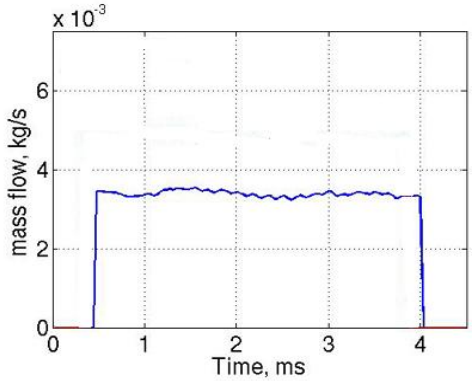


Figure 1: The injection mass flow rate profile of the single-hole injector under consideration

IV. RESULTS AND DISCUSSION

The outcome regimes from the droplet collision, including bouncing, separation, coalescence and defragmentation, have obviously great effects on predicting the spray tip penetration. Hence, the droplet collision must be modeled in the numerical computations. Figure 2 shows the importance of the collision modeling in spray numerical calculations.

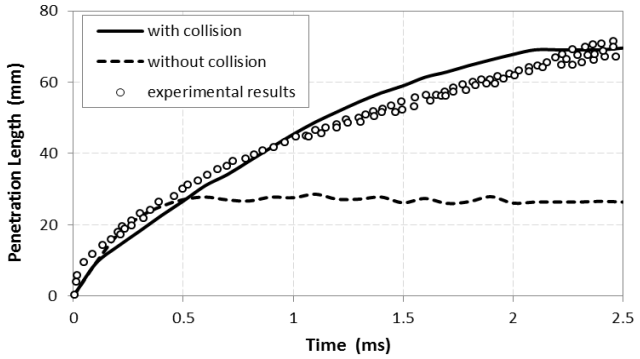


Figure 2: Effect of droplet collision modeling on spray tip penetration

As seen, the case in which the collision of droplets is not considered greatly underestimates the spray penetration length in compare with the experimental results.

In order to compare the abilities of different breakup models, the enhanced TAB model (ETAB), WAVE breakup model and KHRT breakup model applied to the numerical code to calculate the penetration length (Figure 3). The shapes of the spray obtained from these models are shown in Figure 4 at the end of the injection duration (i.e. 2.5ms after the start of the injection).

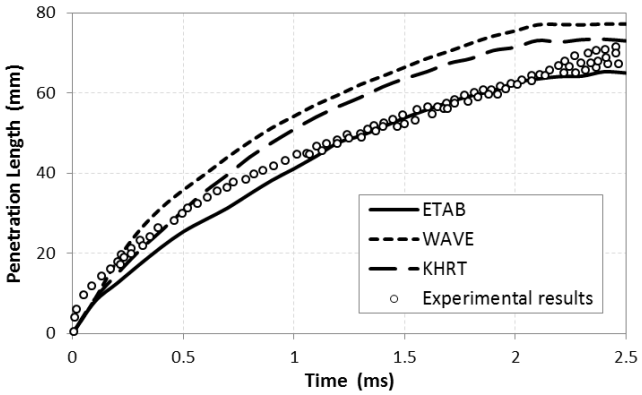
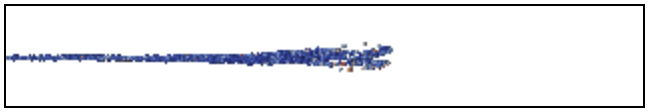
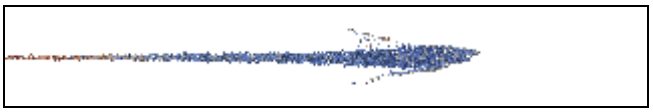


Figure 3: Comparing different breakup models abilities in predicting the spray tip penetration, P_{inj}=600 bar, P_{amb}=50 bar, T_{amb}=683 K, spray angle=15°

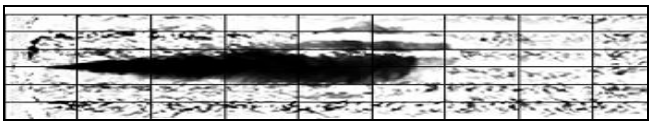


(a) ETAB breakup model



(b) WAVE breakup model

(c) KHRT breakup model



(d) Experimental image of the spray shape

Figure 4: The spray shape at the end of the injection (t = 2.5 ms) presented by a) ETAB model, b) WAVE model, c) KHRT model and d) experimental result by Chalmers HP/HT spray rig

It is noticed that the ETAB model best predicts the penetration length and the shape of the spray, especially when approaches to the end of the injection duration.

As turbulence plays an important role in droplets interaction, standard k-ε turbulence model, its modified version which mentioned before and Lander Sharma k-ε

model (Launder and Sharma, 1974) are applied to the simulations and compared with the experimental results.

As seen in Figure 5, the modified k-ε and especially the Lander Sharma k-ε turbulence models very accurately predict the spray tip penetration. Therefore, the combination of ETAB breakup model and Lander Sharma k-ε turbulence model with considering the collision effects is applied to the simulations henceforth.

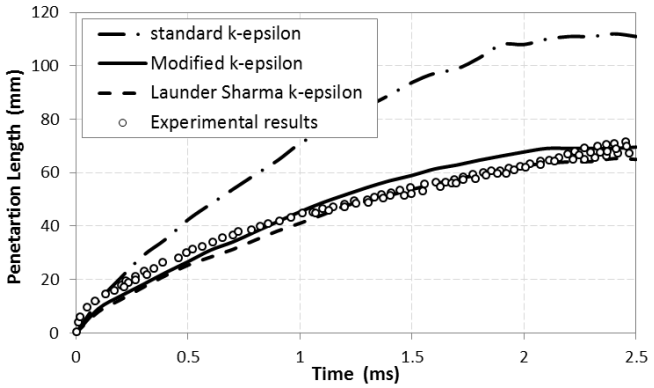


Figure 5: Comparing different turbulence models abilities in predicting the spray tip penetration, (P_{inj}=600 bar, P_{amb}=50 bar, T_{amb}=683 K, spray angle=15°)

Now that the appropriate model for simulating the spray process is detected, the thermodynamics effects, including injection and ambient pressure and temperatur, on penetration length are investigated.

A. Effects of Ambient Properties

The properties of the ambient in which the fuel is injected play an important role in the spray characteristics. For instance, the lower the ambient pressure, the easier the fuel droplets can diffuse into the gas ambient which consequently results in longer penetration length. This fact is illustrated in Figure 6 and 7 by plotting the penetration length in different ambient pressures.

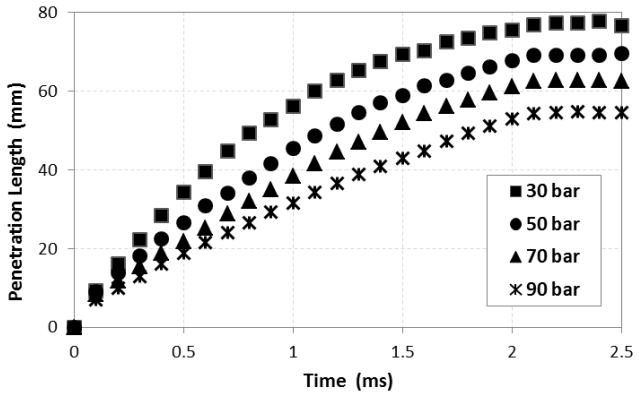


Figure 6: Spray tip penetration variation with time for different ambient pressures, (P_{inj}=600 bar and T_{amb}=683 K)

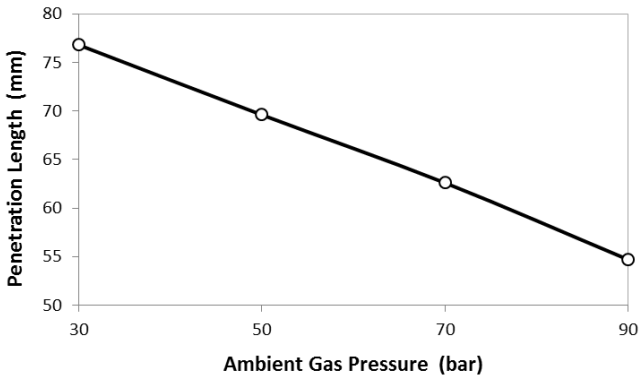


Figure 7: Spray tip penetration variation versus ambient pressure, (P_{inj}=600 bar and T_{amb}=683 K)

Changes in the injection ambient temperature cause the aerodynamic forces on the droplets varied and also make the properties of the droplets change, which consequently influence on the spray tip penetration. In Figure 8 the penetration length variation during injection is plotted for different ambient temperatures. Figure 9 also shows the penetration length variation versus ambient gas temperature.

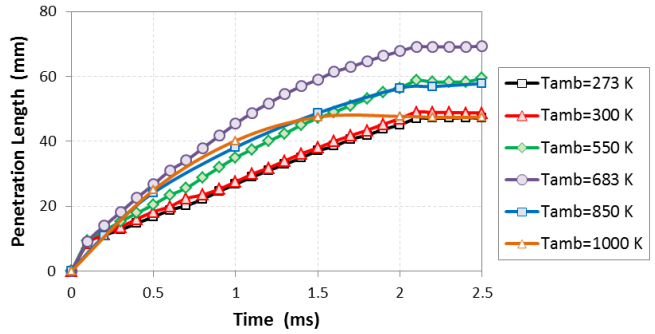


Figure 8: Spray tip penetration variation with time for different ambient temperatures, (P_{inj}=600bar and T_{inh}=320K, P_{amb}=50bar)

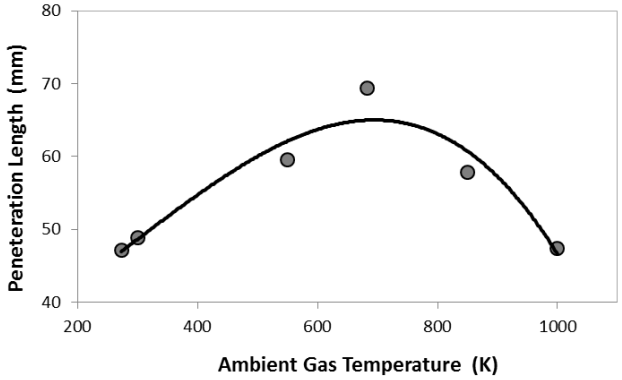


Figure 9: Spray tip penetration variation versus ambient temperature, (P_{inj}=600bar and T_{inh}=320K, P_{amb}=50bar)

As illustrated in Figures 8 and 9, spray penetration length begins to increase with an increase in ambient temperature (up to about 700K) due to decrease in the droplet density and increase in the droplets kinetic energy and consequently its better penetration into the gas ambient. However, further

increases in ambient temperature causes the evaporation rate of droplets increase and show the dominant influence on the spray penetration length and makes it decrease.

B. Effects of Injection Properties

Figure 10 demonstrates the variation of penetration length during the injection time for different injection pressures.

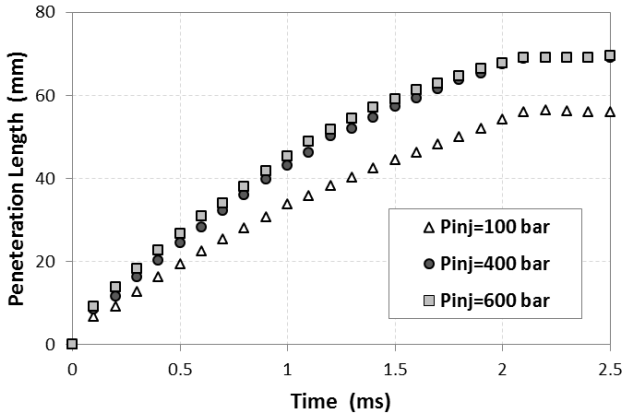


Figure 10: Spray tip penetration variation with time for different injection pressures, (P_{amb}=50 bar and T_{amb}=683 K)

It is recognized that increase in injection pressure leads into increase in spray tip penetration due to rise in the initial spray momentum.

Figure 11 shows the variation of penetration length versus injection pressure.

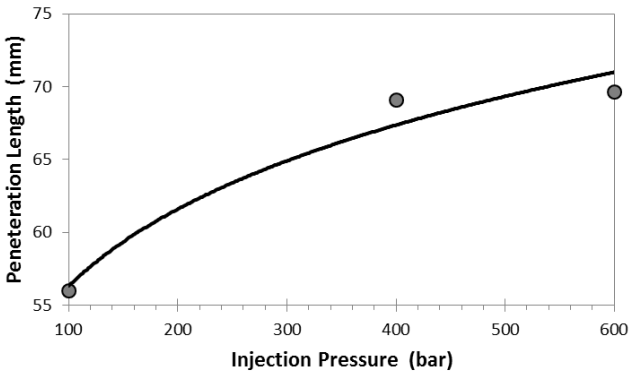


Figure 11: Spray tip penetration variation versus injection pressure, (P_{amb}=50bar and T_{amb}=683 K)

The influence of injection temperature on spray tip penetration is shown in Figures 12 and 13.

It is understood that increase in the injection temperature makes the kinetic energy of the droplets rise and hence results into the increase in the penetration length up to around 330K (i.e. near the evaporation point). Thereafter the spry tip penetration decreases due the dominant effect of evaporation. However, as magnified in Figure 13, injection temperature does not have significant effect on spry penetration length (i.e. an increase of 140K in the injection temperature only yields 10mm variation in spray tip penetration).

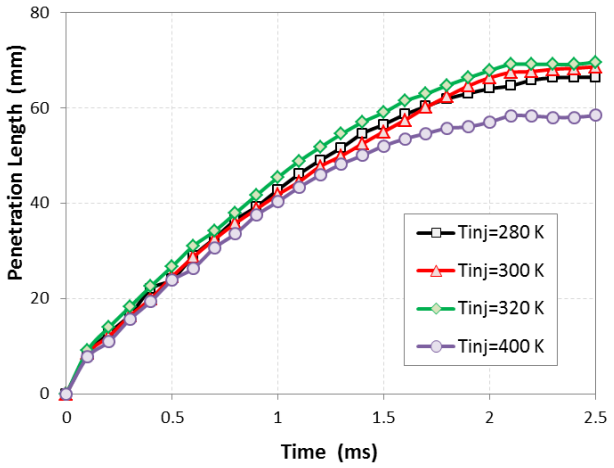


Figure 12: Spray tip penetration variation with time for different injection temperatures

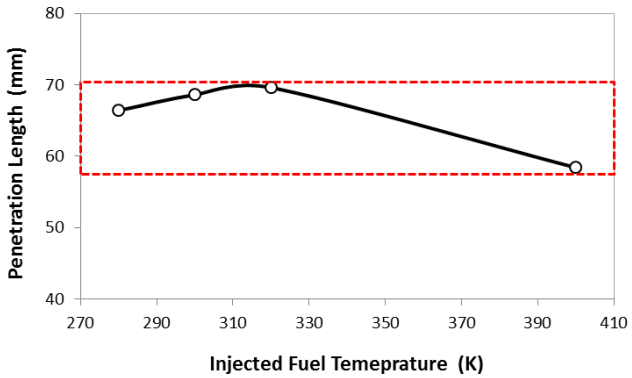


Figure 13: Spray tip penetration variation versus injection temperature

V. CONCLUSION

Modeling the collision in spray simulation is of great importance due to dependence of the spray tip penetration on the droplet collision outcome regimes.

ETAB breakup model and Lander Sharma k-ε turbulence model with considering the collision effects are recognized to be an appropriate combination for studying the spray behavior, especially spray tip penetration.

Investigating the effects of thermodynamic properties showed that increase in injection pressure leads into increase in spray tip penetration due to rise in the initial spray momentum, while adverse effect occurs when the ambient pressure increased.

Ambient temperature shows a dual effect on the spray penetration length. At first, increase in the ambient temperature makes the density of the droplets decrease and increase their kinetic energy, which consequently yields an increase in the spray tip penetration. However, further increase in ambient temperature makes the droplet evaporation dominant and results to a decrease in the penetration length.

Results shows that the effect of injection temperature on the penetration length has a similar trend to the ambient temperature effect, but it is not significant so much.

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