

Simulation and Modeling of the Spray Characteristics of Biodiesel and Ammonia Mixtures Carbon-Neutral Fuel

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Abstract: The purpose of this research is to employ computational fluid dynamics to identify the properties of the spray generated during the spray biodiesel simulation (CFD). The variables under investigation were spray angle, penetration, and area. In the constant volume chamber, biodiesel is used as the fuel for combustion. Different levels of ambient pressure and temperature were used during the simulation. Variable ambient pressure levels of 4 MPa, 6 MPa, and 8 MPa were used. At the same time, the ambient temperature was fixed to 850 K. The results demonstrate that the biodiesel spray angle increased at high ambient pressure. The findings also showed that as ambient temperature rose, the length of the spray and the spray area shrank. Fuel in the constant volume chamber vaporised at a rapid rate as a result of the rise in ambient temperature.

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1. Introduction

Fuel consumption for energy sources to the engine combustion system is increasing every day, following the increase in vehicles every day. Nowadays, there are more than half a billion fleets and commercial vehicles, a number that is expected to grow at a rate of 3% annually and double in the next 20 years [1-5]. As a result, many researchers have made studies on alternative fuels that can be used on vehicles and

can also reduce emissions that can cause pollution. In addition, there are other factors that can potentially reduce engine emissions such as flow in the cylinder, combustion process, chemical kinetics, engine geometry, fuel-air mixture formation, spray, and others [6-8]. These factors are also being studied to find ways to reduce emissions and decrease the negative impact on the environment. Alternative fuels, such as natural gas, hydrogen, propane, ethanol, methanol, and butanol derived from vegetable and waste-derived oils, are used in motor vehicles to deliver direct propulsion, with the goal of causing less damage to the environment or reducing

air pollution compared to conventional fuels. These fuels are often prescribed by regulations as a way to reduce emissions. Biofuels, such as biodiesel made from animal fats or vegetable oils, are considered a renewable source of energy. However, only a small percentage of biofuels are currently used as an alternative fuel. Another alternative fuel is ammonia, which has zero emissions and can reduce pollution [9-10].

Biodiesel-Ammonia is the alternative fuel that focusing in this study. As a fuel that can replace petroleum, biodiesel-ammonia has numerous benefits, such as the fact that ammonia emits no carbon dioxide because it is carbon-free, has three hydrogen atoms and one nitrogen atom, and is easily detectable due to its distinct odour, making leaks simple to find [11-13]. Research has been done on the air mixing that causes diesel spray ignite and its connection to higher exhaust emissions. Diesel engines are regarded as effective thermodynamic engines in the automobile sector. To keep up with the changes brought about by the growing number of vehicles on the road, technological breakthroughs, and expanding development, it is essential to research ways to make diesel engines better. The findings of this study could enhance fuel efficiency and maintain cleaner engines.

Efforts have been made to reduce hazardous emissions from diesel engines through technological innovation and expansion [6-9]. One method for expanding diesel engines is through a better fuel-air mixture and fuel droplet atomization. Development and innovation in high-pressure injection technology can provide a good fuel-air mixture and produce fine atomization. Research on spray penetration and fuel distribution is crucial to understand the effect of high injection pressure spray. The geometry of the injection nozzle plays a crucial role in this research, as it can provide insight into the spraying characteristics and formation of the fuel-air mixture

The importance of sprays in commercial and scholarly research due to their wide range of uses and inherent multiphase phenomena that occur in them. High efficiency and low pollution combustion in direct injection diesel engines can be greatly aided by spray optimization. Ambient flow parameters such as pressure [4], temperature [5], and shape of the flow field in the combustion chamber [6] have an impact on spray formation and development, which in turn affects mixture formation in the chamber. Droplet velocities are predicted to decrease as the spray angle increases. Ultra-high injection of the sprays has been used to produce higher levels of atomization to improve mixture formation, taking into account the impacts of chamber geometry and fuel type [7] [8].. The impact of several classical and hybrid break-up models on the production and break-up of the spray are also investigated [9]. Computational simulations are increasingly being used as a primary analytical tool in engine research to validate experimental findings and offer designers updated data.

This study aims to evaluate how high ambient temperatures affect spray characteristics of biodiesel fuel by employing Computational Fluid Dynamics (CFD) software. Fuel injectors are mounted in this study with injector nozzle 6-holes at an angle of 15° and an orifice diameter of 0.129 mm. Additionally, the ambient pressure within the combustion

chamber were varied and were 4 MPa, 6MPa and 8MPa. The ambient temperature and injection pressure were both maintained at 850 K and 100 MPa, respectively.

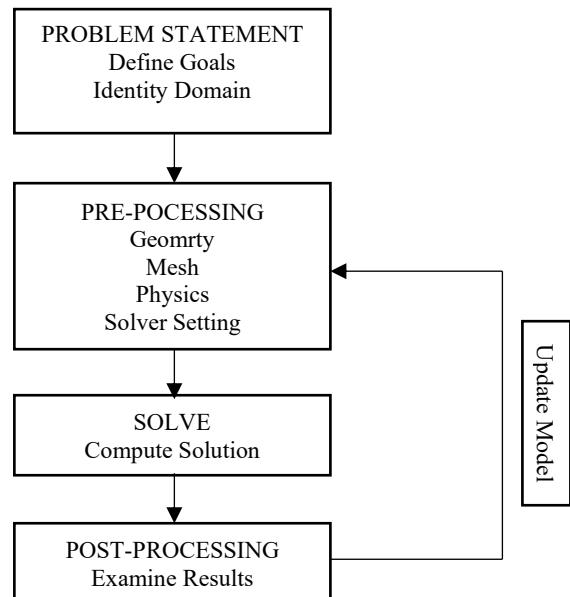


Figure 1: Flowchart of Methodology

1. Simulation

Pre-processing, solver stage, and post-processing were the three main stages of the simulations of biodiesel spray conducted in this study using Ansys Fluent. Furthermore, only the combustion chamber, fuel, and injector nozzle were considered in the simulations. The injector will have a total of 6 nozzle holes, each with an angle of 15°. An experimental design approach will be employed to determine the geometry of the nozzle, specifically a nozzle length of 2 mm and a nozzle diameter of 0.129 mm. The procedure for conducting this study objective is shown in Figure 1. The rapid compression machine (RCM) combustion chamber and nozzle injector cross sections shows in Figures 2, as well as the injectors geometry with six orifice holes, are depicted in 3D models shows in Figure 3. The section geometry inside the combustion chamber is schematically shown in Figure 4. This illustration shows a 1/2 part of the injector's overall geometry for its six nozzle orifices. For the aim of conducting a simulation analysis, the observation of the 1/2 portion is both acceptable and sufficient. This illustration shows a half-section of the injector's overall geometry, which includes nozzle orifices. For the purposes of simulation study, the observation of 1/2 segment is adequate.

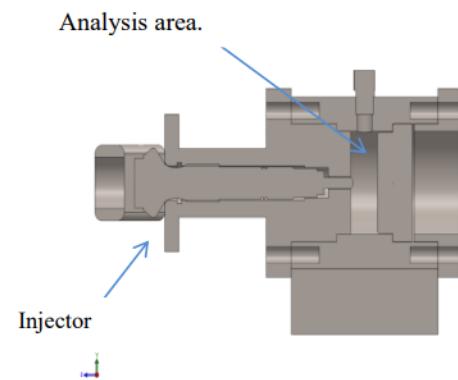


Figure 2: Combustion chamber and The injector's orifice holes

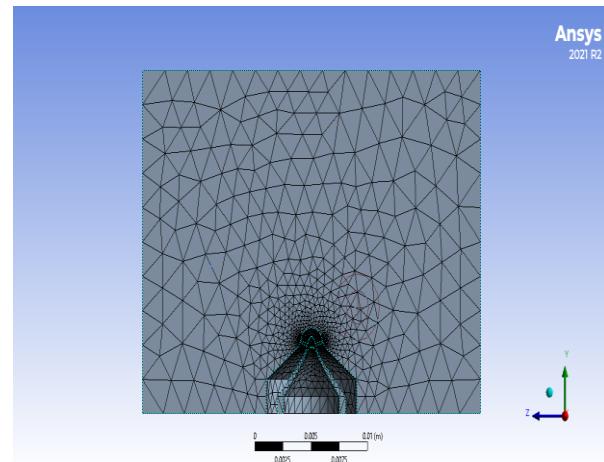


Figure 4: Meshing geometry of nozzle injector

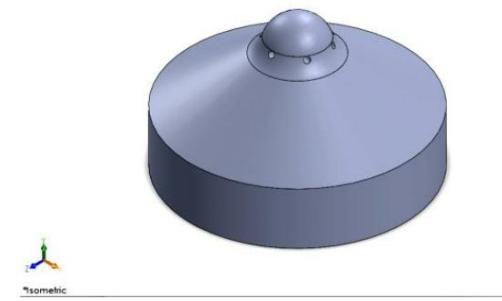


Figure 3: nozzle injector cross section

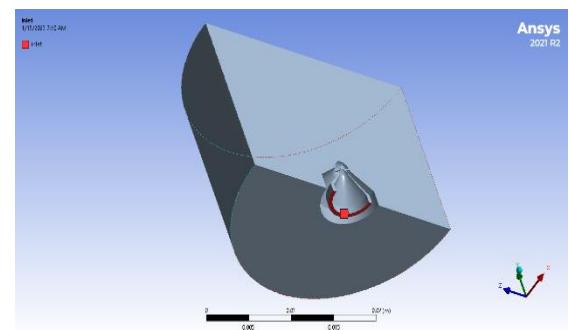


Figure 6: The nozzle injector inlet

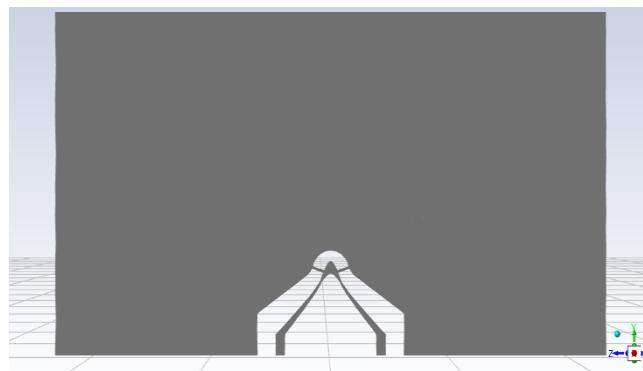


Figure 4: Cross section of an injector-equipped combustion chamber

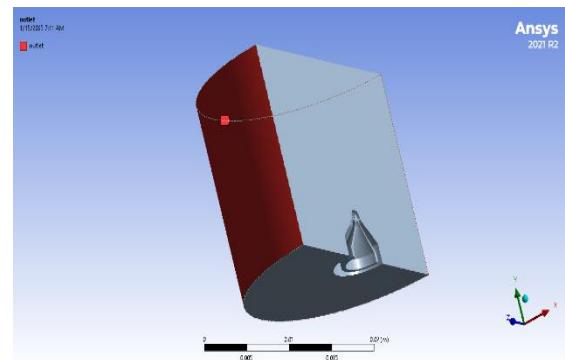


Figure 7: The nozzle injector outlet

Figure 5 illustrates the produced mesh used in this simulation. As a result, the inlet, outlet, combustion chamber wall, and injector were employed as the study's boundary conditions. These are illustrated in Figures 6 to 8. In the meantime, boundary conditions are employed in ANSYS Fluent to replicate the fuel injection system activities displayed in Table 1.

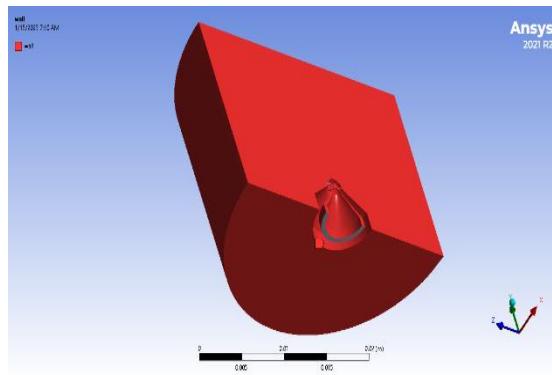


Figure 8: The nozzle injector wall

Table 1: Boundary condition of ANSYS Fluent

General	Pressure based with absolute velocity formulation	Transient time
Model	Species transport	Air-Biodiesel
Viscous	k-epsilon	Realizable
Material	Air	Ammonia
Boundary Condition	inlet	Outlet Wall
	Ambient Temperature	850 K
Operating Parameter	Ambient pressure	4 MPa 6 MPa 8 MPa
	Injection pressure	10 MPa
	Nozzle Injector	0.129 mm

2. Results and Discussion

The research uses CFD simulations to analyze the expansion of fuel spray in order to evaluate the quality of new fueling equipment. The simulations were run by adjusting the biodiesel-ammonia mixture, density, and ambient pressure to avoid spray ignition. The results are presented in table 2 to table 4 and images that show the comparison of the spray creation process at different times and under different conditions. The images show the spray velocity, which is lowest near the chamber wall and zero at the wall due to the no-slip boundary condition.

Table 2: Image formation of spray contour for biodiesel-ammonia, A2 (2%NH₃+98%B30)

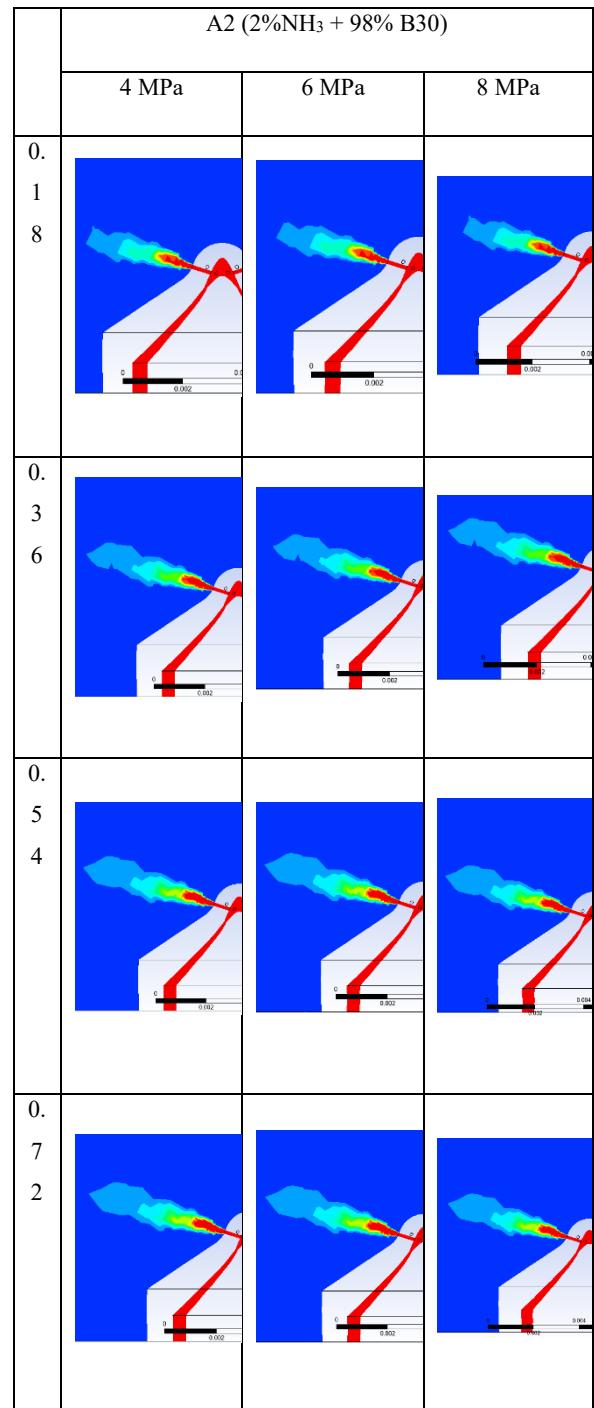


Table 3: Image formation of spray contour for biodiesel-ammonia, A4 (4%NH₃+96%B30)

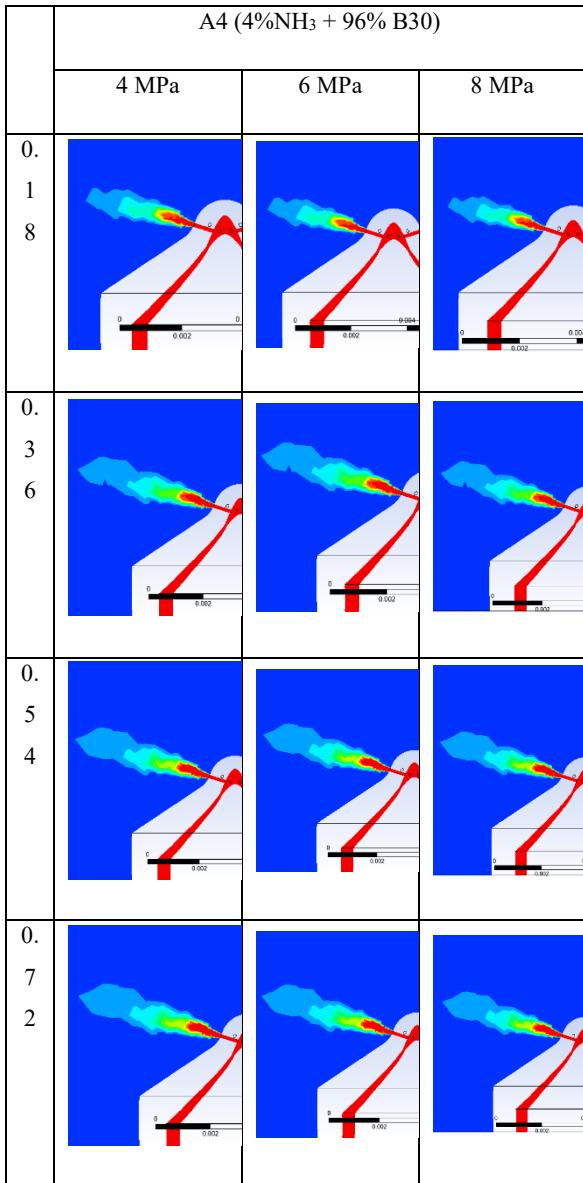
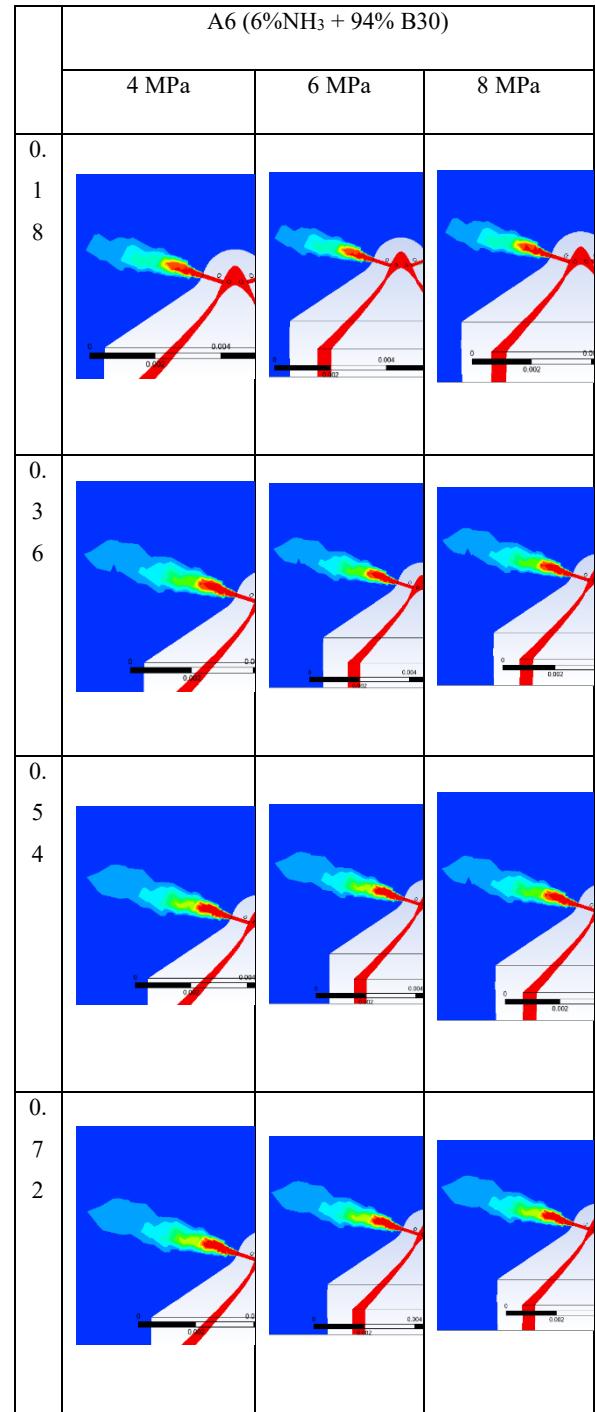


Table 4: Image formation of spray contour for biodiesel-ammonia, A6 (6%NH₃+94%B30)



The contour shows variations in spray velocity, with the highest velocity in the red portion and lowest in the blue portion. The no-slip boundary condition at the chamber wall causes the velocity to be 0 m/s close to the wall. The spray contour is also affected by ambient pressure and density, with increased pressure and density resulting in a decrease in ignition delay and increased heat capacity at the spray boundary

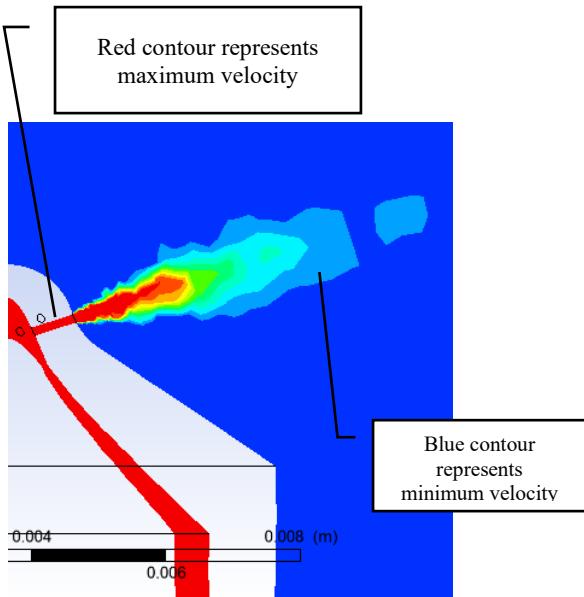


Figure 9: Simulating visual penetration flow through a single orifice

The length of penetration for a biodiesel-ammonia fuel mixture is shown to be affected by temperature and density conditions. As shown in Figure 10 to 12, the penetration length fluctuates in response to changes in ambient pressure and density. The findings indicate that pressure and ambient density have an impact on the spray penetration length, with higher pressures resulting in greater penetration. The ambient temperature also affects the length of penetration, with increased air density causing the spray penetration to vary. Ammonia is more sensitive to temperature changes. The simulation is fixed at a temperature of 850 K and the effort to compensate for the slow ammonia flame speed, considerable boost pressure and compression ratio are needed. Ammonia may be successfully used in dual-fuel mode with diesel in compression-ignition engines.

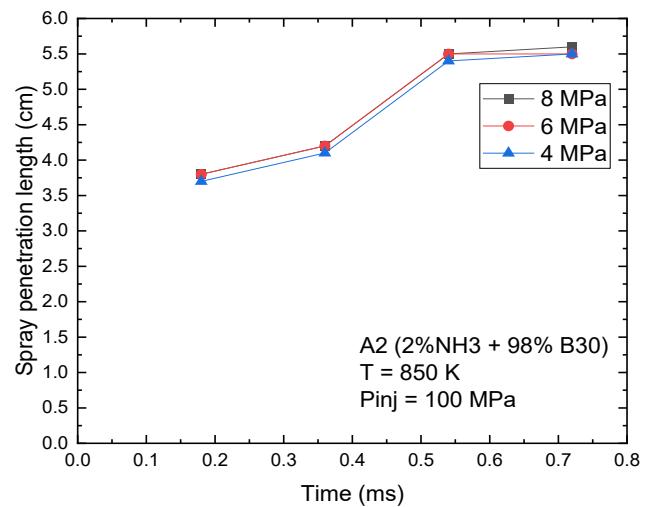


Figure 10: The graph of spray penetration length against the time of the spray from the injector for biodiesel-ammonia A2.

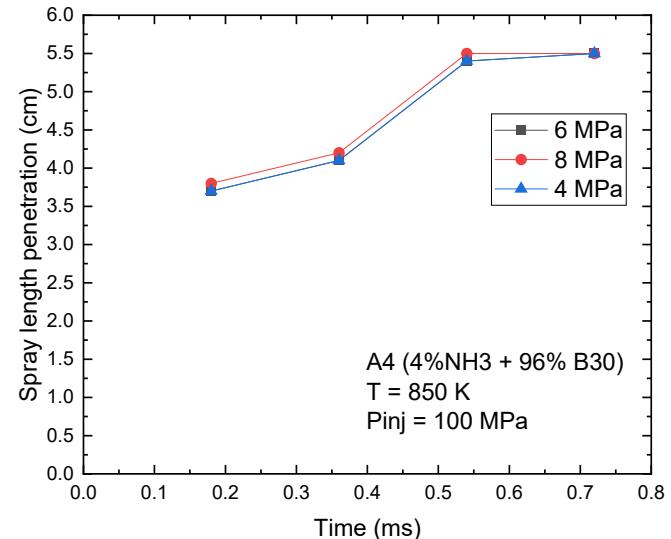


Figure 11: The graph of spray penetration length against the time of the spray from the injector for biodiesel-ammonia A4

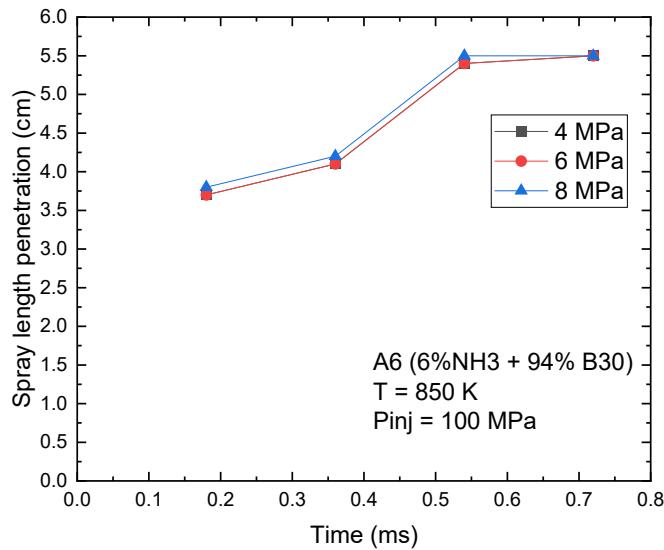


Figure 12: The graph of spray penetration length against the time of the spray from the injector for biodiesel-ammonia A6

The droplet size diameter and velocity distributions in spray are important characteristics for the analysis, design, operation and optimization of practical spray systems. The particle diameter is found to be constant across all parameters, from the nozzle's outlet to the walls. The findings indicate that pressure and ambient density have an impact on particle diameter and droplet size, smaller droplet size particles exist closer to the spray tip, the higher the ambient density value. Figure 13 to 15 shows that the spray's angle is also affected by ambient pressure and density, with discrepancies in ambient pressure, and injector pressure. The spray was resisted by the ambient density at an angle that was shorter the lower the pressure differences between the injector and ambient were. The vector and contour that can be used to determine the spray cone angle by measuring the spray angle's amplitude.

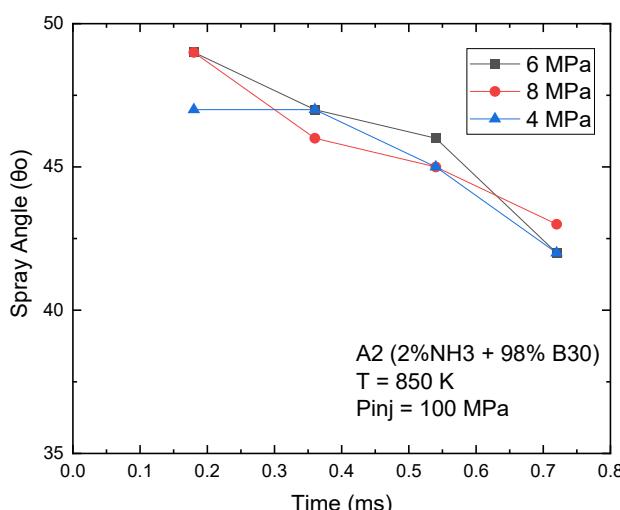


Figure 13: The graph of spray angle against the time of the spray from the injector for biodiesel-ammonia A2

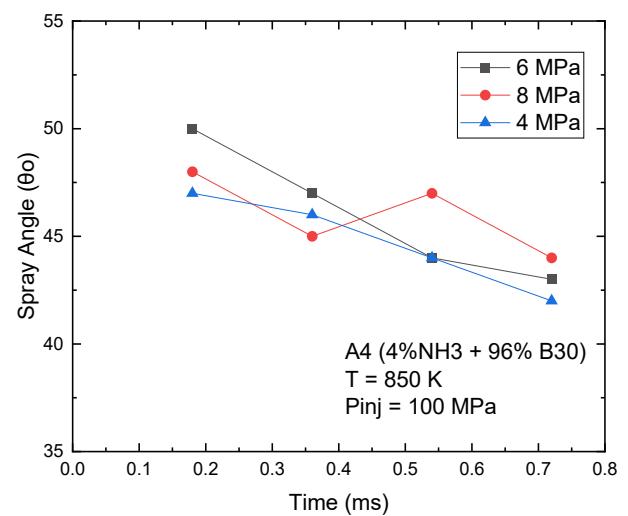


Figure 14: The graph of spray angle against the time of the spray from the injector for biodiesel-ammonia A4

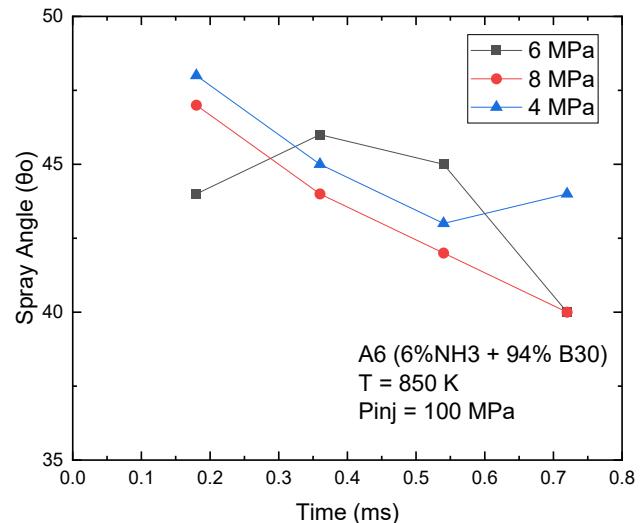


Figure 15: The graph of spray angle against the time of the spray from the injector for biodiesel-ammonia A6

3. Conclusion

The chapter examines the impact of temperature and density conditions on the penetration length of a biodiesel and ammonia fuel mixture using a simulation with a half orifice. Results show that variations in ambient pressure and injector pressure have an effect on the spray penetration length and spray angles. The study found that the ambient pressure has a correlation with the expanding spray penetration length, with higher pressures resulting in greater penetration. The length of penetration is projected to be significantly influenced by ambient temperature. The study also found that the spray's particle size is constant from the nozzle's outlet to the walls and that the pressure and ambient density have an impact on the spray's angle. The study concludes that accurate information about droplet diameter and velocity distributions in spray is essential for the design, operation, and optimization of spray systems and that the pressure and ambient density have a significant impact on particle diameter and spray angle.

Additionally, the study finds that variations in ambient pressure, injector pressure and temperature have an effect on the spray penetration length, and that ambient pressure, temperature and density have an effect on the droplet size and spray angle. The effects of high ambient pressure sprays are also investigated in combustion chamber engine geometry using a simplified nozzle.

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- [10] G. A. B. R. M. a. B. R. Fukuda K., "An Open Cycle Simulation of DI Diesel Engine Flow Field Effect on Spray Processes," SAE Paper, p. 696, 2012.
- [11] G. A., "Numerical Simulation of Ultra-High Injection Diesel and Biodiesel Fuel Sprays," Electronic Theses and Dissertation, 2012.
- [12] G. A. B. R. a. B. R. M. Fukuda K., "Numerical Investigation of Spray Characteristics of Diesel Alternative Fuels," SAE Paper, 2012.
- [13] D. M. a. G. A., "Investigation of Jet Break-Up Process in Diesel Engine Spray Modelling," Journal Applied Science, vol. 9, pp. 2078-2087, 2009.

References

- [1] H. C. M. T. & M. H. Ong, "A review on energy pattern and policy for transportation sector in Malaysia," *Renewable and Sustainable Energy Reviews*, pp. 532-543, 2012.
- [2] Khalid, A., Ja'at, N., Johari, A. M., & Maheswaran, K. (2019). Investigation on the Flame Propagation of Ethanol-Gasoline Blend in Different Ambient Pressure in a Constant Volume Chamber. *Fuel, Mixture Formation and Combustion Process*, 1(1).
- [3] D. E. Ibrahim Dincer, "A perspective on the use of ammonia as a clean fuel: Challenges and solutions," *International Journal of Energy Research*, pp. 4827-4834, 2020.
- [4] Mohamed Sunar, N., Abdullah, N. F. N., Anak Gani, P., Matias Peralta, H. M., & Khalid, A. (2019). Potential of Biofuel from Extraction of Microalgae Biomass via Domestic Wastewater Phytoremediation. *Fuel, Mixture Formation and Combustion Process*, 1(1).
- [5] Khalid, A., Ja'at, N., Mohd Johari, A., & Maheswaran, K. (2019). Investigation on the Flame Propagation of Ethanol – Gasoline Blend in Different Ambient Pressure in a Constant Volume Chamber. *Fuel, Mixture Formation and Combustion Process*, 1(1).
- [6] Mohd Sahabudin, M. A. S., & Razali, M. A. (2019). Effect of Material Composition Towards Flame Spread Behavior of Flammable Materials from Pineapple Fibre and Paper. *Fuel, Mixture Formation and Combustion Process*, 1(2).
- [7] Radzali, M. H., Hakim Zulkifli, A. F., Khalid, A., Radzali, M. H., & Jacob, D. W. (2020). Effect of Methanol-Gasoline Blend and Ambient Pressure on Flame Propagation and Exhaust Emission of Spark Ignition (SI) Engine. *Fuel, Mixture Formation and Combustion Process*, 2(2).
- [8] L. a. R. I. T. C., "Effect of Ambient Pressure on," *International Journal of Multiphase Flow*, vol. 3, pp. 904-920, 2007.
- [9] P. S. H. J. a. L. C. S. Kim H., "Comparison of Experimental and Predicted Atomization Characteristics of High-pressure Diesel Spray Under Various Fuel and Ambient Temperature," *Journal of Mechanical Science and Technology*, vol. 24, no. 7, pp. 1491-1499, 2010.