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Analysis of Spray Droplet Nozzle Characteristics on Biodiesel (B35) with Injection Pressure Variations

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Abstract. This study, entitled *Analysis of Spray Droplet Characteristics of Nozzle in Biodiesel (B35) under Injection Pressure Variations*, investigates the effect of injection pressure on the spray droplet atomization characteristics of Biodiesel B35 and correlates these characteristics with changes in fuel molecular composition determined using Gas Chromatography–Mass Spectrometry (GC–MS). The novelty of this research lies in integrating spray atomization analysis with GC–MS-based molecular characterization to explain how molecular composition influences fuel atomization behavior. An experimental approach was employed using several injection pressure variations in a nozzle system, followed by GC–MS analysis of Diesel B0, Biodiesel B35, and the B0+B35 blend. The GC–MS results revealed that the blended fuel exhibited a broad molecular weight distribution ranging from 106.165 to 843.6107 g/mol, containing both light hydrocarbons, such as O-xylene (C_8H_{10}), and heavy hydrocarbons, such as hexacontane ($C_{60}H_{122}$). Biodiesel B35 showed the highest average molecular weight due to the predominance of fatty acid methyl ester (FAME) compounds, whereas Diesel B0 exhibited the lowest molecular weight because of its higher proportion of light hydrocarbon fractions. The blending process also resulted in stable, reduced, disappeared, and newly formed molecular species, indicating changes in molecular distribution caused by physical interactions between the fuels. These compositional changes affected key fuel properties, including viscosity, volatility, and atomization performance. Spray image analysis demonstrated that increasing injection pressure produced finer and more uniformly distributed droplets, indicating improved atomization quality. The findings demonstrate that the interaction between fuel molecular characteristics and injection pressure plays a significant role in determining spray behavior and has the potential to improve diesel engine combustion efficiency and fuel performance.

Keywords : Biodiesel B35, Diesel B0, GC-MS, spray droplet, injection pressure, atomization, nozzle..

1. INTRODUCTION

Current advances in diesel engine technology increasingly demand improved combustion efficiency and reduced exhaust emissions. Diesel engines remain one of the most widely used power generation systems in the transportation, industrial, agricultural, and power generation sectors because of their high thermal efficiency, reliability, and durability [1]. However, diesel engines are also significant sources of particulate matter (PM), carbon monoxide (CO), unburned hydrocarbons (HC), and nitrogen oxides (NOx), all of which contribute to environmental degradation and adverse human health effects [2]. Consequently, the development of cleaner alternative fuels and the optimization of fuel injection systems have become major research priorities aimed at achieving higher combustion efficiency while meeting increasingly stringent emission regulations [3]. In Indonesia, the mandatory implementation of Biodiesel B35, consisting of 35% fatty acid methyl ester (FAME) blended with 65% petroleum diesel, has been fully implemented since 2023 as part of the national strategy to reduce dependence on fossil fuels, improve energy security, and lower greenhouse gas emissions. The nationwide B35 program has substantially increased biodiesel utilization, making Indonesia one of the world's largest biodiesel consumers and producers [3], [4]. Although B35 offers significant environmental and economic benefits, its higher viscosity, density, and molecular weight compared with conventional diesel fuel alter spray atomization characteristics, fuel-air mixing, and combustion performance. These changes highlight the importance of understanding the relationship between the molecular composition of Biodiesel B35 and its spray characteristics under different injection pressures, thereby providing scientific support for optimizing diesel engine performance and fuel injection systems [4–6].

One effort to reduce the environmental impact of diesel engine use is the use of biodiesel as an alternative fuel. Biodiesel, such as B35, is a blend of fossil diesel fuel and fatty acid methyl ester (FAME)-based biodiesel[4]. The use of biodiesel not only aims to reduce dependence on fossil fuels but also to improve lubrication properties and lower overall carbon emissions[3], [4]. Biodiesel has different physical characteristics than conventional diesel, such as higher viscosity, greater density, and lower volatility. These differences can affect the injection and combustion processes in a diesel engine's combustion chamber[5], [6]. One crucial aspect of a diesel engine system is the fuel injection process through the nozzle. This process significantly determines the quality of fuel atomization, which is the process of breaking down liquid fuel into small droplets that mix with air before combustion occurs[7]. Atomization quality is greatly influenced by injection pressure, nozzle design, and the physical properties of the fuel used. The better the atomization process, the greater the contact surface area between the fuel and air, allowing for faster and more complete vaporization and combustion.Injection Pressure (IP) is a key factor influencing spray droplet characteristics[6], [7], [8]. Increasing injection pressure generally results in smaller droplet sizes and a more homogeneous spray distribution. This occurs because the greater kinetic energy breaks down the fuel stream into finer particles. Conversely, lower injection pressure tends to produce larger droplets and uneven distribution, which can reduce combustion efficiency[6], [8].

In addition to pressure, the chemical composition of the fuel also significantly influences the atomization process. Diesel B0 and Biodiesel B35 blends have different molecular characteristics, both in terms of carbon chain length and oxygen content in their molecular structures[4], [5]. Diesel B0 is dominated by aliphatic hydrocarbons with high volatility, while Biodiesel B35 contains ester compounds with longer carbon chains and oxygen-rich properties[9], [10]. These differences cause changes in physical properties such as viscosity, density, and surface tension, which ultimately affect the spray droplet formation process at the nozzle.Based on Gas Chromatography–Mass Spectrometry (GC-MS) testing results, the blend of Diesel B0 and Biodiesel B35 exhibits a fairly broad molecular distribution, with the presence of light to heavy compounds. This indicates that the blend is not simply a simple combination but also undergoes changes in molecular distribution due to physical interactions between the components[10]. Light compounds, such as O-xylene, play a role in the initial evaporation process, while heavy compounds, such as hexacontane, affect viscosity and atomization. These differences in molecular characteristics directly impact the fuel's combustion properties[11].

Changes in molecular composition due to blending also indicate the presence of compounds that remain constant, are reduced, are lost, and are formed. This phenomenon indicates that the blending process is not simply a physical process but also affects the chemical distribution within the blend[11], [12], [13]. The dominance of hydrocarbons in diesel and the contribution of ester compounds in biodiesel create intermediate fuel characteristics, somewhere between those of pure diesel and pure biodiesel.In the context of an injection system, these changes in the physical and chemical properties of the fuel have a direct impact on spray droplet characteristics[12], [13], [14]. Fuels with higher viscosity tend to produce larger droplets, resulting in less optimal atomization. Conversely, fuels with high volatility evaporate more easily and form a more homogeneous mixture with air. The combination of injection pressure variations and fuel type is a crucial factor in determining combustion quality[14], [15].

Based on this description, a more in-depth analysis is needed regarding the relationship between injection pressure variations and spray droplet characteristics in B35 biodiesel, as well as how changes in fuel molecular composition affect the atomization process[16], [17]. To address this gap, the present study integrates GC–MS-based molecular characterization with spray droplet analysis under various injection pressures. The novelty of this research lies in establishing the relationship between changes in fuel molecular composition, particularly in Biodiesel B35 and its blends, and the resulting spray atomization characteristics. By combining chemical and spray analyses within a single experimental framework, this study provides a more comprehensive understanding of the mechanisms governing fuel atomization. The findings are expected to contribute to the optimization of diesel fuel injection systems, support the development of more efficient and environmentally friendly diesel engines, and provide scientific guidance for the wider application of biodiesel fuels in modern diesel engine technology.

2. METHODS

This study employed an experimental research approach to investigate the effect of injection pressure variations on spray droplet characteristics in a diesel fuel system using Biodiesel B35, Diesel B0, and their blends[18]. The experimental method was selected because it allows direct observation of cause-and-effect relationships between controlled variables (injection pressure and fuel type) and the resulting response variable (spray droplet characteristics)[16], [17], [18]. The study was conducted under controlled laboratory conditions to ensure consistency and repeatability of results.

Research Approach and Design

The research design used in this study is a quantitative experimental design. The independent variables include injection pressure variations and fuel type (Diesel B0, Biodiesel B35, and B0+B35 blend). The dependent variable is the spray droplet characteristics, which include droplet diameter and spray pattern distribution. Controlled variables include nozzle type, ambient temperature, and test setup configuration to minimize external influences on the results.

Population and Sample

The population in this study refers to all possible spray characteristics generated by diesel injection systems under varying operating conditions[18], [19]. The sample consists of spray droplets produced from a test nozzle system using three types of fuel: Diesel B0, Biodiesel B35, and a 1:1 mixture of both fuels (50 ml Diesel B0 and 50 ml Biodiesel B35). Each fuel sample was tested under multiple injection pressure conditions to obtain comparative data on spray droplet behavior.

Operational Definition of Variables

Injection pressure is defined as the pressure applied to force fuel through the nozzle during the injection process, measured in bar or MPa[2], [3], [5]. Fuel type refers to the composition of the tested fuel, namely Diesel B0, Biodiesel B35, and their mixture. Spray droplet characteristics are defined as the physical attributes of the atomized fuel, including droplet diameter size, distribution pattern, and spray dispersion quality. Smaller droplet diameters indicate better atomization quality, which contributes to improved combustion efficiency.

Data Collection Methods

Data collection was conducted using an experimental test rig consisting of a fuel injection system, high-pressure pump, nozzle, and pressure gauge. Fuel was injected through the nozzle under controlled pressure variations[9], [10]. The resulting spray was captured using a high-speed imaging system combined with proper lighting to ensure clear visualization of droplet formation. The recorded images were then analyzed using image processing techniques to determine droplet size and distribution.

Additionally, chemical composition data of the fuels were obtained using Gas Chromatography–Mass Spectrometry (GC-MS) analysis. This method was used to identify molecular composition, molecular weight distribution, and chemical changes in Diesel B0, Biodiesel B35, and their blends. The GC-MS data provided supporting information to explain differences in physical spray characteristics based on fuel molecular structure.

Data Analysis Method

The experimental data were analyzed using quantitative and descriptive statistical methods. Spray images were processed using digital image analysis software to determine droplet size distribution under each injection pressure and fuel type [11], [12]. Prior to analysis, the images were calibrated using a reference scale, converted into grayscale, and segmented using an intensity threshold to identify individual droplets. The equivalent droplet diameter was then calculated for each test condition, and the average droplet size together with its distribution was used to evaluate atomization performance.

Each experimental condition was repeated to ensure measurement consistency, and the results are presented as mean values. GC–MS analysis was performed under controlled operating conditions using helium as the carrier gas, with the injector operated in split mode and the oven temperature programmed from a low initial temperature to a higher final temperature to separate compounds with different boiling points [9], [10]. The obtained chromatograms and mass spectra were analyzed by comparing the detected peaks with the reference library to identify molecular species and determine their relative abundances. The analysis focused on molecular weight distribution, dominant compounds, and compositional changes among Diesel B0, Biodiesel B35, and the blended fuel samples. The relationships between fuel molecular characteristics, including molecular weight, viscosity, and volatility, and spray droplet behavior were evaluated by comparing the experimental results obtained under different injection pressures. Descriptive statistical analysis was employed to identify trends in droplet size variation and atomization quality, while the combined physical and chemical analyses were used to explain the influence of fuel composition on spray characteristics and their implications for diesel engine combustion performance.

3. RESULTS AND DISCUSSION

3.1 GC-MS Test of Diesel B0 + Biodiesel B35

Gas Chromatography–Mass Spectroscopy (GC–MS) testing on a mixture of Diesel B0 + Biodiesel B35 fuel was carried out to identify the chemical composition of compounds and understand the changes in molecular distribution due to the mixing process of the two fuels. This analysis aims to provide a comprehensive picture of the molecular characteristics of the mixture, which is a combination of aliphatic hydrocarbons from diesel and ester compounds (fatty acid methyl esters/FAME) from biodiesel[12], [13]. The B0+B35 mixture has chemical properties that are not simply the sum of each component, but also show changes in compound distribution due to physical interactions and differences in volatility properties. Therefore, the use of the GC–MS method is very important to separate and identify each component based on the retention time and the resulting mass fragmentation pattern. Through this test, it is expected to determine the dominance of the type of compound in the mixture, changes in the amount or loss of certain compounds, and the range of molecular weights formed. This information is the basis for understanding the effect of fuel composition on physical properties, such as viscosity and volatility, as well as its implications for the atomization and combustion processes in diesel engines, as seen in Figure 1 below.

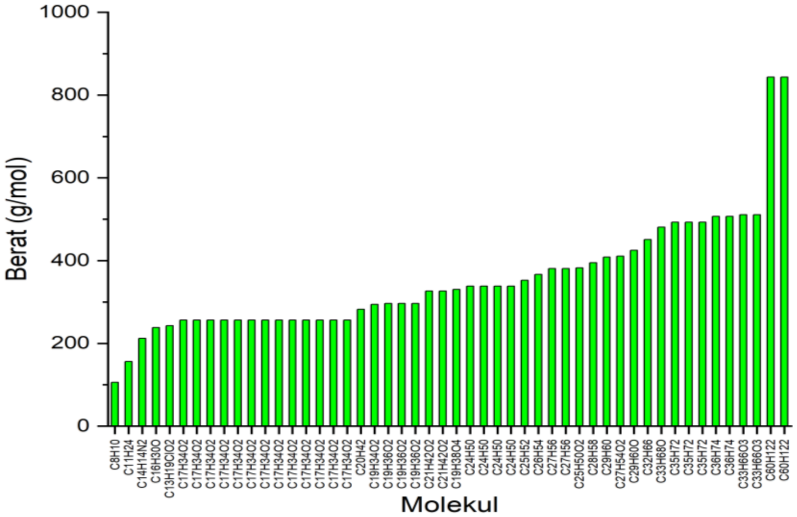


Figure 1 GC-MS Test Results of Diesel B0 + Biodiesel B35

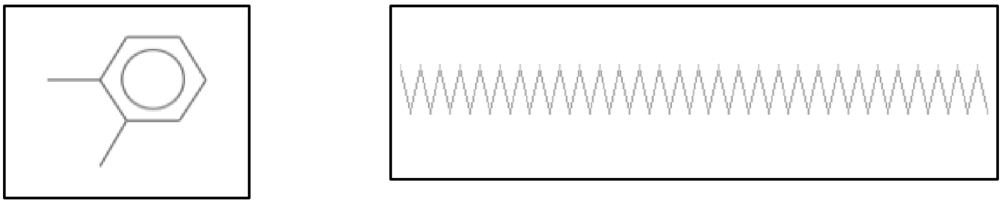
The results of GC-MS testing of Diesel B0 Biodiesel B35 fuel showed the lowest molecular weight of O-Xylene C_8H_{10} = 106.165 grams/mol, while the highest molecular weight of Hexacontane $C_{60}H_{122}$ = 843.6107 grams/mol. Based on Figure 1, the results of Gas Chromatography–Mass Spectroscopy (GC–MS) testing on the Diesel B0 + Biodiesel B35 fuel mixture showed a fairly wide molecular weight distribution. The compound with the lowest molecular weight was identified as O-xylene (C_8H_{10}) with a value of 106.165 g/mol, while the compound with the highest molecular weight was hexacontane ($C_{60}H_{122}$) with a value of 843.6107 g/mol. The presence of O-xylene as a light aromatic compound indicates the presence of volatile fractions in the fuel mixture. This compound has a relatively low boiling point, making it crucial for the initial evaporation process and the formation of the air-fuel mixture. This light fraction supports better atomization and accelerates ignition during combustion.

The presence of hexacontane, a very long-chain hydrocarbon, indicates the presence of a heavy fraction with low volatility[4], [5]. This compound tends to increase fuel viscosity and slow the evaporation process. In a combustion system, the heavy fraction can cause delayed atomization, larger droplet formation, and the potential for residue or deposit formation. The broad molecular distribution of the B0+B35 blend reflects a combination of characteristics between pure diesel and biodiesel. The B0 diesel contributes light to medium hydrocarbon fractions, while the B35 biodiesel contributes to an increase in long-chain compounds and oxygenates. As a result, this blend has intermediate properties in terms of both volatility and viscosity. Overall, the GC-MS results indicate that:

a) The B0+B35 mixture has a wide molecular weight range (±106–843 g/mol)
b) Contains a combination of light aromatic compounds and heavy hydrocarbons
c) The fuel's characteristics are intermediate between diesel and biodiesel.

The implication of these results is that the fuel mixture has a balance between ease of evaporation (from the light fraction) and energy stability (from the heavy fraction). The increase in heavy fractions can also affect the atomization and combustion processes, which is in line with the results of previous tests related to droplet size. Thus, this GC–MS analysis provides an important basis in understanding the relationship between molecular composition and fuel performance in a diesel engine system. Based on the results of the GC–MS analysis of the

Diesel B0 + Biodiesel B35 fuel mixture, compounds with a fairly contrasting molecular weight range were identified, namely C_8H_{10} as the light fraction and $C_{60}H_{122}$ as the heavy fraction. The C_8H_{10} compound is an aromatic hydrocarbon with a relatively low molecular weight, which is included in the group of volatile compounds. The presence of this compound indicates that the fuel mixture still contains light fractions that play an important role in the initial evaporation process. This fraction supports faster formation of the air-fuel mixture and increases the ease of ignition during the combustion process. In contrast, the compound $C_{60}H_{122}$ is a very long-chain hydrocarbon with a high molecular weight included in the heavy fraction. This compound has low volatility and tends to increase fuel viscosity. Its presence can affect the atomization process by producing larger droplets and slowing the fuel evaporation process in the combustion chamber. The significant difference between the two compounds shows that the B0+B35 mixture has a wide molecular distribution, reflecting a combination of characteristics of pure diesel and biodiesel. The light fraction of diesel contributes to increased volatility, while the heavy fraction of biodiesel increases the content of long-chain molecules, as seen in Figure 2 below.



C_8H_{10} **$C_{60}H_{122}$**

Figure 2. Results of GC-MS (Gas Chromatography-Mass Spectrometry) testing

The results of the GC-MS (Gas Chromatography-Mass Spectrometry) test showed that the average molecular weight was highest for B35 biodiesel, followed by the B0+B35 mixture, and the lowest for B0 diesel fuel. The results of the Gas Chromatography–Mass Spectrometry (GC–MS) test showed differences in the distribution of average molecular weights for each type of fuel tested. Based on this analysis, it was found that B35 biodiesel had the highest average molecular weight, followed by the B0+B35 mixture, and the lowest was B0 diesel fuel. The higher average molecular weight value in B35 biodiesel was due to the dominance of fatty acid methyl ester (FAME) compounds which have long carbon chains and contain oxygen groups in their molecular structure. These compounds generally have a larger molecular mass than the hydrocarbons that make up diesel, thus increasing the overall average molecular weight of biodiesel. In the B0+B35 mixture, the average molecular weight value is between the two, which indicates intermediate properties due to the combination of hydrocarbon compounds from diesel and ester compounds from biodiesel. The decrease in the average molecular weight compared to B35 occurs due to dilution by B0 diesel which has lighter molecular components. B0 diesel has the lowest average molecular weight because it is dominated by aliphatic hydrocarbon compounds with relatively shorter carbon chains and does not contain oxygenate groups. This causes the properties of diesel fuel to be lighter and have higher volatility. This difference in average molecular weight has direct implications for the physical properties and performance of the fuel, including:

a) B35 biodiesel tends to have higher viscosity and lower volatility
b) B0 diesel has higher volatility and better atomization
c) B0+B35 blends exhibit intermediate characteristics

The results of GC-MS (Gas Chromatography-Mass Spectrometry) confirm that increasing the biodiesel content in fuel will increase the average molecular weight, which in turn affects the atomization process, droplet formation, and combustion efficiency in the diesel engine system, as seen in Figure 3 below.

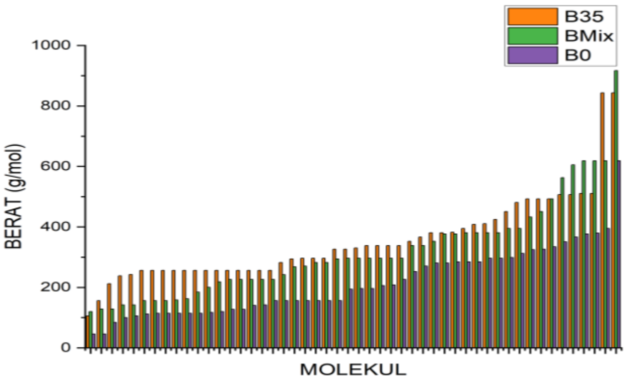


Figure 3 Molecular Weight of GC-MS Test Results of Biodiesel B0, B35 and Bmix

Figure 3 shows the molecular weight distributions from GC-MS analysis of three types of fuel: B0, B35, and Bmix. In general, the graph shows that all samples experienced an increase in molecular weight from the light compound fraction to the heavy compound fraction. This reflects variations in carbon chain length in each fuel, with low molecular weight compounds being at the beginning of the graph, while high molecular weight compounds were at the end. B0, which is pure diesel fuel without biodiesel blends, shows a tendency for lower molecular weight values compared to B35 and Bmix. This indicates that B0 is dominated by hydrocarbon compounds with relatively shorter carbon chains. This characteristic makes B0 more volatile and has a better atomization process during combustion. This dominance of light compounds can also have an impact on environmentally unfriendly emissions, such as increased hydrocarbon (HC) and carbon monoxide (CO) emissions.

In contrast to B0, B35 shows the highest molecular weight value among the three samples, especially in the heavy compound fraction at the end of the graph[6], [7], [8]. This is due to the 35% biodiesel content, which generally consists of long-chain fatty acid methyl esters (FAME). The presence of these compounds increases the average molecular weight of the fuel. Consequently, B35 tends to have a higher viscosity and slower evaporation rate than B0. This fuel has the advantage of cleaner and more stable combustion, as well as lower emissions, making it more environmentally friendly. Bmix exhibits characteristics that fall between B0 and B35. Its molecular weight is neither as low as B0 nor as high as B35, indicating that this blend composition produces a more balanced distribution of compounds between light and heavy fractions[5], [6], [13]. This provides the advantage of a combination of properties, maintaining adequate atomization while improving combustion quality and reducing emissions. Bmix can be considered an optimal compromise between engine performance and environmental aspects.

In the heavy fraction section, a significant increase was observed in B35, followed by Bmix, and then B0. This phenomenon confirms that the higher the biodiesel content in the mixture, the greater the contribution of heavy compounds in the fuel[9], [10]. These heavy compounds generally come from long carbon chains that play a role in increasing the lubricity value of the fuel and combustion stability. The analysis results show that increasing the biodiesel content in the fuel mixture is directly proportional to the increase in the average molecular weight. This has a positive impact on reducing emissions and improving combustion quality, but also needs to be balanced with attention to the physical properties of the fuel such as viscosity and atomization ability. Selecting the right mixture composition is an important factor in optimizing fuel performance while maintaining environmental aspects, as seen in Figure 4 below.

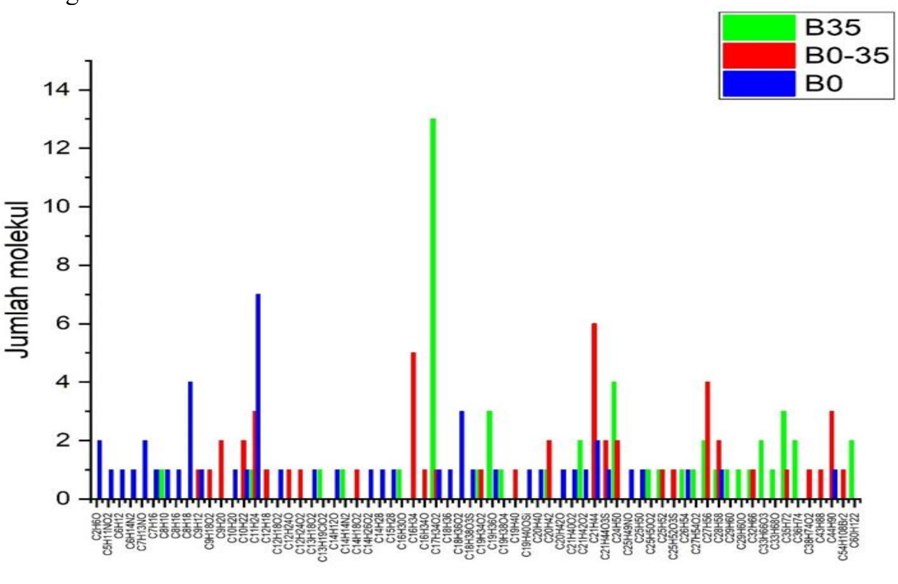


Figure 4 Changes in Molecular Compounds of Biodiesel B0, B35 and Bmix

Based on the results of GC-MS analysis. The horizontal axis represents the type of compound (generally hydrocarbons and their derivatives with varying carbon chain lengths), while the vertical axis shows the number of molecules or the intensity of the compound's appearance in the sample[12], [13], [14]. The graph shows that each fuel has different molecular composition characteristics. In B0 (blue), the distribution of compounds tends to be more even but with a relatively low to moderate number of molecules in almost all fractions. This indicates that pure diesel is dominated by a mixture of hydrocarbons with a fairly wide distribution, but no single type of compound is very dominant. This composition is common in fossil fuels consisting of various hydrocarbon fractions, ranging from short to medium chains. In B35 (green), there is a significant spike in certain types of compounds, indicated by peaks in the number of molecules that are much higher than in B0. This indicates the dominance of certain compounds, which are most likely methyl ester compounds (FAME) resulting from biodiesel. These compounds usually have a long carbon chain structure (e.g., C_{16}–C_{18}) and appear in greater amounts due to the relatively high composition of biodiesel (35%). This dominance indicates that the addition of biodiesel not only increases the molecular weight (as seen in Figure 3) but also significantly changes the chemical composition of the fuel by increasing the concentration of certain compounds.

B0-35 (red) shows a distribution pattern that falls between B0 and B35. The number of molecules in some compounds increases compared to B0, but not as much as B35. This indicates that this blend produces a more balanced composition between hydrocarbons from diesel and esters from biodiesel. The absence of extreme dominance of any one compound indicates that B0-35 has a more homogeneous blend, potentially providing more stable combustion characteristics than B0, without the excessive increase in viscosity as in B35. This change in the number of molecules significantly impacts the physical and chemical properties of the fuel. In B35, the dominance of ester compounds tends to increase the fuel's viscosity, density, and lubrication properties. The oxygen content in biodiesel molecules also contributes to more complete combustion, thereby reducing emissions of harmful gases such as carbon monoxide and unburned hydrocarbons. On the other hand, the dominance of certain compounds can also lead to uneven evaporation characteristics.

In B0, although the compound distribution is more even, the absence of oxygen in the hydrocarbon molecules tends to result in incomplete combustion, potentially increasing emissions. Meanwhile, in B0-35, the combination of the two compounds provides a balance between combustion performance and the fuel's physical properties, making it an optimal alternative for diesel engine applications. Figure 4 shows that increasing the biodiesel content in a fuel blend not only affects the molecular weight but also significantly alters the distribution and dominance of the chemical compounds within it. These changes directly impact combustion characteristics, energy efficiency, and emissions, making selecting the right blend composition crucial for developing efficient and environmentally friendly fuels.

A. Fixed Molecules

Based on Figure 4, the results of GC-MS testing of molecular compounds that do not change (remain) in B35 biodiesel mixed with B0 diesel fuel are: $C_{19}H_{34}O_2$, $C_{25}H_{52}$, $C_{32}H_{66}$ and the results of GC-MS testing, there are several compounds that do not experience changes (remain present) when B35 biodiesel is mixed with B0 diesel fuel, namely $C_{19}H_{34}O_2$, $C_{25}H_{52}$, and $C_{32}H_{66}$. The presence of these compounds in both B0, B35, and their mixtures indicates that these compounds are stable and not significantly affected by the mixing process. The $C_{19}H_{34}O_2$ compound is a group of fatty acid esters (Fatty Acid Methyl Ester/FAME) which generally comes from biodiesel. Its constant presence indicates that the main components of biodiesel do not experience degradation or further chemical reactions when mixed with diesel fuel. This indicates that the blending process between B35 and B0 is physical (physical mixing), not a chemical reaction that changes the molecular structure. Meanwhile, $C_{25}H_{52}$ and $C_{32}H_{66}$ are saturated hydrocarbon compounds (long-chain alkanes) that generally come from the heavy fraction in diesel (B0). The fact that these compounds remained detectable after blending indicates that the hydrocarbon components of diesel also did not experience changes in chemical structure during the blending process. The presence of these compounds has several important implications. First, it confirms that blending biodiesel and diesel does not damage the main components of each fuel, so that the basic properties of both are still maintained. Second, the stability of these compounds indicates good compatibility between biodiesel and diesel, which is important to ensure optimal engine performance. Third, the presence of ester and hydrocarbon compounds together in the blend provides a combination of properties, such as improved lubricity of biodiesel and combustion characteristics of diesel.

B. Molecules Reduce and Disappear

The molecular composition of B35 biodiesel, after being mixed with B0 diesel, changes occur, with some molecules being reduced or lost. The same molecular composition, but with a reduced quantity, is: $C_{17}H_{34}O_2$, $C_{24}H_{50}$, $C_{35}H_{72}$. While the missing molecular compounds are C_8H_{10}, $C_{13}H_{19}C_lO_2$, $C_{14}H_{14}N_2$, $C_{16}H_{30}O$, $C_{19}H_{36}O$, $C_{19}H_{38}O_4$, $C_{21}H_{42}O_2$, $C_{25}H_{50}O_2$, $C_{26}H_{54}$, $C_{27}H_{54}O_2$, $C_{29}H_{60}$, $C_{29}H_{60}O$, $C_{33}H_{66}O_3$, $C_{33}H_{68}O$, $C_{36}H_{74}$, $C_{60}H_{122}$. The results of the molecular composition analysis showed that B35 biodiesel experienced changes in its chemical structure after being mixed with B0 diesel fuel. This change was indicated by a decrease in the number of several molecular compounds and the loss of certain components in the B0+B35 mixture. This phenomenon indicates the occurrence of physical interactions and the possibility of changes in component distribution during the mixing process. Molecular compounds that were still detected but experienced a decrease in number included C17H34O2, $C_{24}H_{50}$, and $C_{35}H_{72}$. These compounds are generally part of the main structure of biodiesel and long-chain hydrocarbons. The decrease in intensity or amount can be caused by the dilution effect of B0 diesel, so that the relative proportion of the compound becomes smaller in the mixture. There are a number of compounds that are no longer detected after mixing, namely C_8H_{10}, $C_{13}H_{19}ClO_2$, $C_{14}H_{14}N_2$, $C_{16}H_{30}O$, $C_{19}H_{36}O$, $C_{19}H_{38}O_4$, $C_{21}H_{42}O_2$,

$C_{25}H_{50}O_2$, $C_{26}H_{54}$, $C_{27}H_{54}O_2$, $C_{29}H_{60}$, $C_{29}H_{60}O$, $C_{33}H_{66}O_3$, $C_{33}H_{68}O$, $C_{36}H_{74}$, and $C_{60}H_{122}$. The loss of these compounds can be caused by several factors, including:

a) Dilution effect, where the concentration of a compound becomes so low that it is undetectable by the instrument.
b) Differences in volatility, which cause some components to evaporate more easily or not be detected in the test.
c) Interactions between molecules, which allow for changes in the distribution or association of molecules in the fuel mixture.

These changes in molecular composition indicate that blending biodiesel with diesel not only results in a simple mixture, but also affects the distribution of chemical compounds within it. The dominance of hydrocarbons from B0 diesel causes a relative decrease in oxygenate compounds derived from biodiesel. The implications of these changes are quite significant for fuel properties, including:

a) A decrease in oxygenate compound content can affect combustion quality.
b) Changes in carbon chain composition affect fuel viscosity and density.
c) Variations in molecular structure impact the atomization process and droplet size.

This molecular composition analysis strengthens the results of previous FTIR tests, that the B0+B35 mixture has intermediate chemical characteristics influenced by the dominance of diesel hydrocarbons and limited contribution from biodiesel ester compounds.

C. New and Added Molecules

Phenomena that occur after B35 biodiesel is mixed with B0 diesel include the presence of additional molecules and new molecules. These molecules include: $C_{11}H_{24}$, $C_{20}H_{42}$, $C_{27}H_{56}$, $C_{28}H_{58}$ and the newly formed molecules are: C_9H_{12}, $C_9H_{18}O_2$, C_9H_{20}, $C_{10}H_{22}$, $C_{12}H_{18}$, $C_{12}H_{24}O$, $C_{12}H_{24}O_2$, $C_{14}H_{18}O_2$, $C_{16}H_{34}$, $C_{16}H_{34}O$, $C_{19}H_{40}$, $C_{21}H_{44}$, $C_{21}H_{44}O_3S$, $C_{25}H_{52}O_3S$, $C_{38}H_{74}O_2$, $C_{43}H_{88}$, $C_{44}H_{90}$, $C_{54}H_{108}Br_2$

4. CONCLUSION

Based on the experimental results, it can be concluded that both injection pressure and fuel molecular characteristics significantly influence the atomization behavior of Biodiesel B35. GC–MS analysis revealed that the B0+B35 blended fuel exhibited a broad molecular weight distribution ranging from **106.165 to 843.6107 g/mol**, indicating the presence of both light hydrocarbons, such as O-xylene (C_8H_{10}), and heavy hydrocarbons, such as hexacontane ($C_{60}H_{122}$). Biodiesel B35 exhibited the highest average molecular weight due to the predominance of fatty acid methyl ester (FAME) compounds, whereas Diesel B0 contained a larger proportion of lighter hydrocarbon fractions. The blending process also resulted in stable, reduced, disappeared, and newly formed molecular species, demonstrating changes in molecular distribution that influence important fuel properties, particularly viscosity and volatility.

The spray analysis demonstrated that increasing injection pressure produced finer and more uniformly distributed fuel droplets, indicating improved atomization performance and enhanced fuel–air mixing. These findings confirm that the interaction between fuel molecular composition and injection pressure plays an important role in determining spray characteristics and is expected to improve diesel engine combustion efficiency.

The novelty of this study lies in integrating GC–MS-based molecular characterization with spray droplet analysis to establish the relationship between changes in fuel molecular composition and atomization behavior under different injection pressures. This integrated approach provides a more comprehensive understanding of the mechanisms governing biodiesel spray formation than studies that evaluate fuel composition or spray characteristics separately. The findings provide valuable information for optimizing diesel fuel injection systems, improving combustion efficiency, and supporting the wider implementation of Biodiesel B35 in modern diesel engines.

This study is limited to laboratory-scale spray characterization and molecular composition analysis under controlled operating conditions. Engine performance parameters, combustion characteristics, and exhaust emissions were not directly evaluated. Therefore, future studies should incorporate engine performance testing, combustion analysis, emission measurements, and computational fluid dynamics (CFD) simulations to further validate the relationship between molecular composition, spray atomization, and diesel engine performance under actual operating conditions.

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