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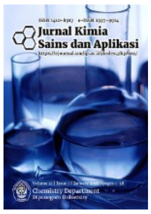

Comparative Study of Volatile Compound Profiles and Fuel Properties of Diesel Blends with *Cymbopogon nardus* and *Cymbopogon citratus* Essential Oils as Natural Bioadditives

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Abstract

The development of environmentally friendly bioadditives has attracted growing attention for improving diesel fuel quality. This study comparatively investigated the role of oxygenated compounds in essential oils from *Cymbopogon nardus* and *Cymbopogon citratus* as natural bioadditives. The essential oils were obtained by hydrodistillation and characterized for yield, moisture content, density, kinematic viscosity, and volatile compound composition using gas chromatography–mass spectrometry. The essential oils were then blended with diesel fuel at five additive concentrations (0.2, 0.4, 0.6, 0.8, and 1.0% (v/v)), with neat diesel (0% (v/v)) serving as the control. The resulting blends were evaluated for density, kinematic viscosity, distillation characteristics, and ignition quality, as indicated by the Calculated Cetane Index (CCI). The results revealed that *C. citratus* essential oil contained a higher proportion of oxygenated compounds than *C. nardus*. The optimal bioadditive concentration was determined to be 0.8% (v/v) for *C. nardus* and 0.6% (v/v) for *C. citratus*, based on a balance between statistically significant CCI improvement and maintaining density and kinematic viscosity within diesel fuel specifications. At these optimal concentrations, the CCI increased from 45.5 for neat diesel to 46.3 for *C. nardus* and to 46.9 for *C. citratus*, respectively, while density and kinematic viscosity remained within diesel fuel specifications. These findings suggest that variations in essential oil composition may contribute to the observed differences in fuel properties and support the potential use of essential oils rich in oxygenated compounds as sustainable bioadditives for diesel fuel applications.

1. Introduction

The increasing demand for diesel fuel has raised significant concerns regarding fuel efficiency, combustion performance, and environmental impact [1]. Diesel fuel remains one of the most widely used energy sources in transportation and industrial sectors due to its high energy density and operational efficiency [2]. However, its combustion characteristics are strongly influenced by physicochemical properties, such as density, kinematic viscosity, and ignition quality, which are closely related to the fuel's chemical composition [3]. Density and kinematic viscosity are important physicochemical properties because they influence fuel injection, spray, atomization, air–fuel mixing, and combustion efficiency in diesel engines [4]. Among these parameters, ignition quality plays a critical role in determining ignition delay, combustion stability, and overall engine performance. It is commonly expressed by the cetane number [5].

In addition to the cetane number, the Calculated Cetane Index (CCI) is widely used as an empirical parameter for estimating diesel fuel ignition quality from density and distillation characteristics [5, 6]. Changes in these properties can significantly affect fuel atomization, spray formation, air–fuel mixing, and combustion behavior inside the engine cylinder [7, 8]. Therefore, improving ignition quality through fuel modification has become a key focus in diesel fuel research.

Conventional strategies to enhance diesel fuel performance typically involve synthetic additives, such as nitrate–based compounds, metal–based additives, and oxygenated fuels. Although effective in improving ignition quality and combustion efficiency, these additives often present several limitations, including high cost, potential corrosion, environmental concerns, and the formation of harmful residues [7, 9, 10, 11]. These drawbacks have driven growing interest in developing renewable and environmentally friendly alternatives.

One promising approach is the use of bioadditives derived from natural products, particularly essential oils. Essential oils have attracted considerable attention as renewable additives because of their high content of oxygenated volatile compounds. Major constituents such as citronellal, citronellol, and geraniol have been reported to facilitate more complete combustion by supplying oxygen during the early stages of fuel oxidation [4, 11, 12, 13]. Previous studies have demonstrated that oxygenated compounds, including monoterpenes and their derivatives, can improve fuel reactivity and combustion characteristics when blended with diesel fuel [13, 14, 15, 16].

Gas chromatography–mass spectrometry (GC-MS) has been widely used to characterize the volatile compound composition of essential oils, enabling the identification of oxygenated compounds that may influence the physicochemical properties of diesel fuel [12, 17]. However, previous studies have mainly employed GC-MS for compositional characterization, whereas the relationships among volatile compound composition, physicochemical properties, and ignition quality remain insufficiently explored. In particular, the use of the CCI as an indirect estimate of cetane number has received limited attention.

C. nardus and *C. citratus* are two plant species widely known for their essential oil content, which differs significantly in chemical composition, particularly in the proportion of oxygenated compounds [18]. Despite their promising characteristics, studies investigating the relationship between volatile compound profiles, physicochemical properties, and ignition quality remain limited. Because *C. citratus* essential oil generally contains a higher proportion of oxygenated compounds than *C. nardus*, it was hypothesized that *C. citratus* would produce greater improvements in diesel fuel properties, particularly ignition quality as indicated by the CCI. Therefore, this study aims to investigate the role of oxygenated compounds in essential oils from *C. nardus* and *C. citratus* and evaluate their potential as bioadditives to improve diesel fuel ignition quality. Furthermore, this study evaluates the relationships among volatile compound composition, physicochemical properties, and CCI to provide deeper insight into the potential of essential oils as sustainable diesel fuel bioadditives.

2. Experimental

2.1. Materials

Fresh leaves of *Cymbopogon nardus* and *Cymbopogon citratus*, B-0 diesel fuel (CN 48), distilled water, and anhydrous magnesium sulfate ($MgSO_4$, Merck) were used in this study.

2.2. Instruments

The main instruments used in this study included a Clevenger-type hydrodistillation apparatus (Duran, Germany), an electric oven (Venticell, Germany), an analytical balance (Sartorius, Germany), a hydrometer (0.800-0.850 g/mL; Alla France, France), a Cannon-Fenske viscometer (SCHOTT Gerate, Germany), a standard ASTM D86 distillation apparatus, and a gas chromatography-mass spectrometry system (GC-MS-QP2010S, Shimadzu, Japan).

2.3. Sample Preparation

Fresh leaves of *Cymbopogon nardus* (L.) Rendle and *Cymbopogon citratus* (DC.) Stapf were collected from Lumajang and Bojonegoro, Indonesia, respectively, and taxonomically identified at the University of Jember. The samples were air-dried for 3 days and then cut into approximately 1-cm pieces before extraction. Diesel fuel was obtained from PPSDM MIGAS Cepu, Indonesia.

2.4. Essential Oil Preparation and Characterization

2.4.1. Moisture Content

Moisture content was determined gravimetrically using a separate subsample that was not subsequently used for hydrodistillation. Approximately 3 g of the sample was placed in a porcelain crucible that had been previously dried at 105°C for 30 min and cooled in a desiccator for 15 min. The sample was then heated in an oven at 105°C for 3 h, then cooled in a desiccator for 15 min before weighing. The heating and weighing steps were repeated until a constant mass was obtained [19]. The moisture content was calculated using Equation 1.

$$Moisture\ content\ (\%) = \frac{w_0 - w_1}{w_0} \times 100\% \quad (1)$$

Where w_0 is the initial mass of the sample and w_1 is the dried mass.

2.4.2. Essential Oil Extraction

Essential oils were extracted by hydrodistillation using a Clevenger-type apparatus. Approximately 275 g (air-dried basis) of plant material was distilled with 2.5 L of distilled water for 3 h. The resulting essential oil was separated from the hydrosol using a pipette [20, 21].

2.4.3. Yield Determination

The yield was calculated based on the ratio of essential oil mass to dried sample mass using Equation 2 [22].

$$Yield\ (\%) = \frac{mass\ of\ essential\ oil}{mass\ of\ dried\ sample} \times 100\% \quad (2)$$

2.5. Diesel Fuel Blend Preparation

Diesel fuel blends were prepared at concentrations of 0.2, 0.4, 0.6, 0.8, and 1.0% (v/v). A total of 150 mL of diesel fuel was mixed with the required volume of essential oil under continuous stirring at 120 rpm for 30 min to ensure homogeneity [23].

2.6. Fuel Property Measurements

2.6.1. Density Measurement

Density was measured using a hydrometer (0.800–0.850 g/mL) in accordance with ASTM D1298-99. All measurements were corrected to the reference temperature of 15°C and performed in triplicate [24].

2.6.2. Kinematic Viscosity

Kinematic viscosity was measured according to ASTM D445-06 using a Cannon-Fenske viscometer at 40°C. Measurements were performed in triplicate, and kinematic viscosity was calculated using Equation 3 [24].

$$v = C \times t \quad (3)$$

Where v is the kinematic viscosity (mm^2/s), C is the viscometer calibration constant (mm^2/s^2), and t is the flow time (s).

2.6.3. Ignition Quality Evaluation

The ignition quality of diesel fuel blends was estimated using the CCI according to ASTM D4737-03 (Standard Test Method for Calculated Cetane Index by Four Variable Equation). Since CCI is an empirical parameter derived from density and distillation characteristics, it provides an indirect estimate of diesel ignition quality rather than a direct measurement of cetane number or ignition delay. The CCI was calculated using density measured according to ASTM D1298-99 and the ASTM D86-01 distillation temperatures corresponding to 10%, 50%, and 90% recovered volume (T_{10}, T_{50}, and T_{90}) [24].

The normalized density (D_N) was first calculated from the measured fuel density (D) using Equation 4.

$$D_N = \mathrm{D} - 0.85 \quad (4)$$

Where D is the fuel density at 15°C (g/mL).

The normalized density was then used to determine the density correction factor (B) according to Equation 5.

$$B = e^{(-3.5D_N)} - 1 \quad (5)$$

Subsequently, the ASTM D86-01 distillation temperatures were normalized using Equations 6-8.

$$T_{10N} = T_{10} - 215 \quad (6)$$

$$T_{50N} = T_{50} - 260 \quad (7)$$

$$T_{90N} = T_{90} - 310 \quad (8)$$

Where T_{10}, T_{50}, and T_{90} are the ASTM D86-01 distillation temperatures corresponding to 10%, 50%, and 90% recovered volume, respectively.

Finally, the calculated values of B, T_{10N}, T_{50N}, and T_{90N} were substituted into Equation 9 to obtain the CCI.

$$CCI = 45.2 + (0.0892)(T_{10N}) + [0.131 + 0.901B](T_{50N}) + [0.0523 - 0.420B](T_{90N}) + 0.00049((T_{10N})^2 - (T_{90N})^2) + 107B + 60B^2 \quad (9)$$

Where CCI is the Calculated Cetane Index; B is the density correction factor, and T_{10N}, T_{50N}, and T_{90N} are the normalized distillation temperatures.

2.7. Gas Chromatography–Mass Spectrometry Analysis

Volatile compound profiles of essential oils and diesel fuel samples were analyzed using GC-MS equipped with a DB-5MS UI capillary column (30 m × 0.25 mm × 0.25 µm). Helium was used as the carrier gas, and electron ionization was operated at 70 eV. For essential oil samples, the injector temperature was set at 250°C, with an oven program of 50°C for 5 min, increased at 5°C/min to 240°C, and held for 17 min. The column flow rate was 0.55 mL/min with a pressure of 13.5 kPa and a split ratio of 129.9:1. For diesel fuel samples, the injector temperature was set at 300°C, with an oven program of 40°C for 5 min, increased at 5°C/min to 300°C, and held for 13 min. The column flow rate was 0.57 mL/min with a pressure of 12.9 kPa and a split ratio of 54.0:1. Mass spectra were recorded over a range of m/z 28-600. Compound identification was performed by comparison of the obtained mass spectra with those in the NIST Mass Spectral Library [25, 26].

2.8. Statistical Analysis

Statistical analysis was conducted to evaluate the effects of essential oil type and concentration on the measured parameters at the 0.05 significance level. A two-way analysis of variance (ANOVA) was used to evaluate the effects of essential oil type, concentration, and interaction. When a significant interaction or main effects were observed ($p < 0.05$), treatment means within each essential oil were compared using one-way ANOVA followed by Fisher's Least Significant Difference (LSD) test.

3. Results and Discussion

3.1. Essential Oil Characteristics and Extraction Performance

Hydrodistillation of *C. nardus* and *C. citratus* successfully produced essential oils with distinct visual appearances. The essential oil of *C. nardus* appeared pale yellow, whereas that of *C. citratus* was darker yellow-brown. Variations in oil color may arise from several factors, including differences in chemical composition, oxidation during processing, or extraction conditions. Therefore, the chemical profile of the oils was further investigated using GC-MS analysis [18, 27]. The measured densities of *C. nardus* and *C. citratus* essential oils were 0.890 and 0.888 g/mL, respectively, which fall within the typical range for lemongrass essential oils. Minor differences in these properties can be attributed to variations in molecular composition, particularly the proportions of oxygenated compounds and higher-molecular-weight constituents, which influence intermolecular interactions [28].

The moisture content of *C. nardus* and *C. citratus* leaves was 68.35% and 74.11%, respectively. Residual moisture plays an important role in hydrodistillation by facilitating cell wall disruption and enhancing mass transfer of volatile compounds into the vapor phase, thereby improving extraction efficiency. The essential oil yield of *C. nardus* (3.37%) was significantly higher than that of *C. citratus* (0.83%), indicating differences in extraction efficiency between the two species. This difference may be attributed to inherent variations in oil gland density and composition. These yields are higher than those reported in previous studies, suggesting that processing parameters such as drying conditions, particle size, and distillation duration significantly influence oil recovery.

3.2. Volatile Compound Profiles of Essential Oils

GC-MS analysis revealed distinct chemical profiles for essential oils of *C. nardus* and *C. citratus* (Figures 1 and 2; Tables 1 and 2). Based on comparison of the obtained mass spectra with the NIST Mass Spectral Library, 48 and 23 compounds were tentatively identified in *C. nardus* and *C. citratus* essential oils, respectively. For clarity of presentation, only compounds with relative abundances greater than 3% are summarized in Tables 1 and 2, whereas the complete chromatograms are shown in Figures 1 and 2. The identified compounds belonged mainly to monoterpene hydrocarbons, oxygenated monoterpenes, sesquiterpene hydrocarbons, oxygenated sesquiterpenes, alkylbenzenes, and other oxygenated compounds.

In *C. nardus* essential oil, *α*-pinene was the most abundant compound (16.21%), followed by geraniol (9.81%), 6-octenal (5.35%), and citronellol (3.64%). Although α-pinene was the most abundant individual compound, the sum of several alkylbenzene derivatives resulted in alkylbenzene being the largest chemical class (49.38%) in *C. nardus* essential oil (Table 3). The predominance of α-pinene observed in this study differs from several reports describing citronellal, citronellol, and geraniol as the major constituents of citronella oil. Such differences may be associated with geographical origin, environmental conditions, harvesting stage, extraction conditions, or chemotype variation, as reported in previous studies [12, 29, 30].

Table 1. Major compounds (> 3%) identified in *C. nardus* essential oils

Compound	Molecular formula	RT (min)	SI	Area (%)
α-pinene	$C_{10}H_{16}$	11.685	96	16.21
Geraniol	$C_{10}H_{18}O$	22.857	94	9.81
6-octenal	$C_8H_{10}O$	19.664	97	5.35
5-Phenylundecane	$C_{17}H_{28}$	33.390	94	4.66
6-Phenyldodecane	$C_{18}H_{30}$	35.662	93	4.42
5-Phenyldodecane	$C_{18}H_{30}$	35.775	94	4.10
Citronellol	$C_{10}H_{20}O$	22.056	96	3.64
(+)-3-carene	$C_{10}H_{16}$	14.535	96	3.49
Tridecane-6-ylbenzene	$C_{19}H_{32}$	37.912	93	3.47
4-Phenylundecane	$C_{17}H_{28}$	33.66	95	3.41
Undecane-2-ylbenzene	$C_{17}H_{28}$	35.147	96	3.36
3-Phenylundecane	$C_{17}H_{28}$	34.212	96	3.28

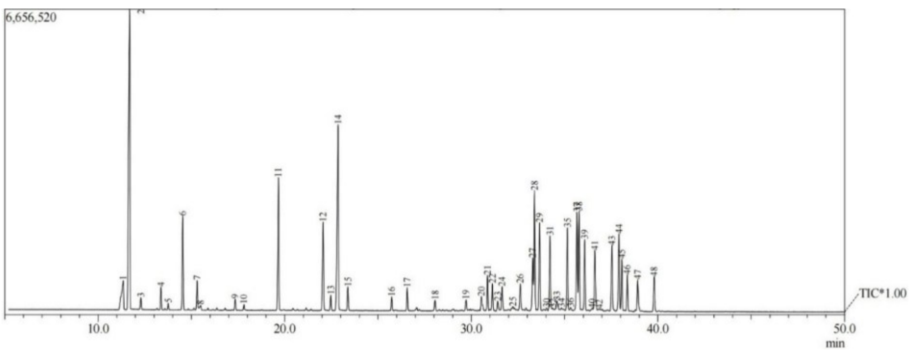

Figure 1. GC-MS chromatogram of *C. nardus* essential oil

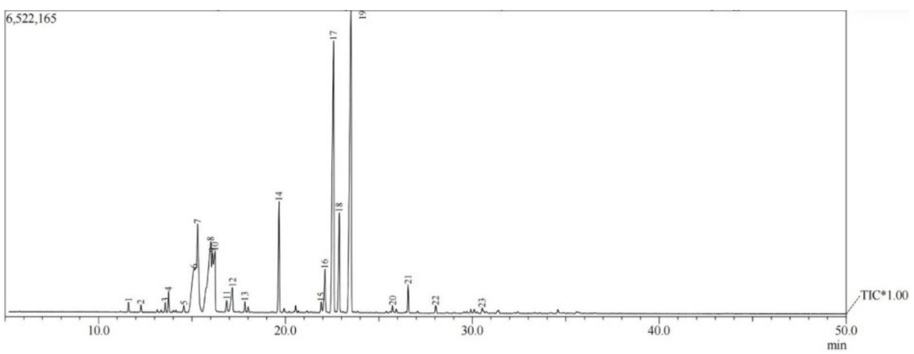

Figure 2. GC-MS chromatogram of *C. citratus* essential oil

Table 2. Major compounds (> 3%) identified in *C. citratus* essential oils

Compound	Molecular Formula	RT (min)	SI	Area (%)
Geraniol	$C_{10}H_{18}O$	23.511	95	24.66
Citronellol	$C_{10}H_{20}O$	22.577	95	20.19
2-(2-Hydroxypropoxy)-1-propanol	$C_6H_{14}O_3$	16.013	96	11.53
1-(2-hydroxypropoxy)propan-2-ol	$C_{10}H_{18}O$	17.838	94	7.95
β-Terpinyl acetate	$C_{12}H_{20}O_2$	15.303	88	7.92
Neral	$C_{10}H_{16}O$	22.886	94	7.89
Linalool	$C_{10}H_{18}O$	19.658	97	4.98
3,3'-oxybis-2-butanol	$C_8H_{18}O_3$	16.237	95	4.45
2-(2-Hydroxypropoxy)propan-1-ol	$C_6H_{14}O_3$	16.104	96	3.14

In *C. citratus* essential oil, geraniol (24.66%) and citronellol (20.19%) were identified as the dominant compounds, followed by β-terpinyl acetate (7.92%), neral (7.89%), and linalool (4.98%). This composition differs from many previous studies reporting citral (geranial and neral) as the predominant constituent of *C. citratus* essential oil. Such variations have been reported in the literature and may be influenced by chemotypic differences, geographical origin, climatic conditions, plant maturity, and extraction parameters [12, 29, 30].

The distribution of chemical classes further highlighted the compositional differences between the two oils (Table 3). To facilitate interpretation, the identified compounds were further classified into monoterpene hydrocarbons, oxygenated monoterpenes, sesquiterpene hydrocarbons, oxygenated sesquiterpenes, alkylbenzenes, and other oxygenated compounds according to their structural characteristics. Oxygenated monoterpenes comprised oxygen-containing monoterpenoid compounds, whereas "other oxygenated compounds" represented oxygenated compounds that do not belong to the terpenoid group. Oxygenated monoterpenes represented the major fraction of *C. citratus* essential oil (70.13%).

In contrast, *C. nardus* exhibited a more heterogeneous composition, with alkylbenzenes constituting the largest chemical class (49.38%), followed by monoterpene hydrocarbons (23.06%) and oxygenated monoterpenes (15.64%). Overall, based on this classification, oxygenated compounds accounted for 97.76% of the identified constituents in *C. citratus* and 25.20% in *C. nardus*. These compositional differences may partially contribute to the observed variations in density, kinematic viscosity, distillation characteristics, and CCI of the fuel blends, owing to the different physicochemical properties of oxygenated and hydrocarbon compounds.

Table 3. Distribution of chemical classes in *C. nardus* and *C. citratus* essential oils

Chemical class	*C. nardus* (%)	*C. citratus* (%)
Monoterpene hydrocarbons (MH)	23.06	1.49
Oxygenated monoterpenes (MO)	15.64	70.13
Sesquiterpene hydrocarbons (SH)	1.95	0.35
Oxygenated sesquiterpenes (SO)	1.12	ND
Alkylbenzenes	49.38	ND
Other oxygenated compounds	8.44	27.28
Total oxygenated compounds	25.20	97.76

ND = not detected

3.2.1. Effect of Essential Oil Addition on Diesel Fuel Properties

Essential oils were applied as bioadditives by blending with diesel fuel (B-0 48) at concentrations of 0– 1.0% (v/v). At these concentrations, all blends appeared macroscopically homogeneous with no visible phase separation (Figure 3), suggesting good miscibility under the experimental conditions. Since the blending process involves simple physical mixing, no chemical reactions are expected to occur. Therefore, the observed changes in fuel properties may be associated with intermolecular interactions between essential oil constituents and diesel hydrocarbons.

Nonpolar compounds such as α-pinene are proposed to interact predominantly through London dispersion forces, whereas oxygenated compounds such as geraniol, citronellol, and other oxygenated constituents may introduce localized polarity, potentially enabling dipole-induced dipole interactions, with limited hydrogen-bonding interactions being possible. These proposed interactions may influence molecular packing and fluid microstructure, which may subsequently affect the macroscopic properties of the fuel blends. A schematic illustration of the proposed intermolecular interactions is presented in Figure 4. The proposed interaction mechanism is presented solely as a conceptual interpretation of the observed changes in fuel properties and should not be regarded as direct experimental evidence.

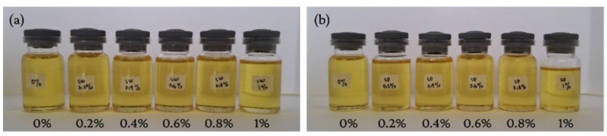

Figure 3. Diesel fuel blends with essential oils at various concentrations: (a) *C. nardus* and (b) *C. citratus*

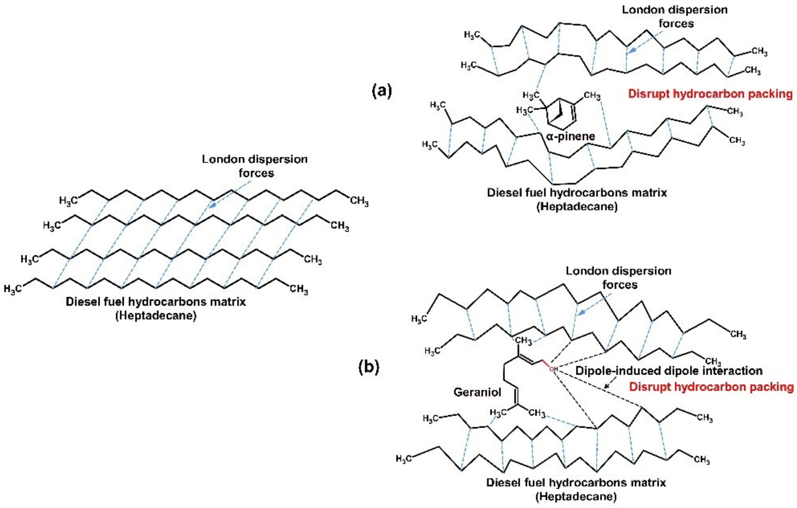

Figure 4. Proposed conceptual illustration of possible intermolecular interactions between the diesel hydrocarbon matrix and essential oil components. Adapted from [13]

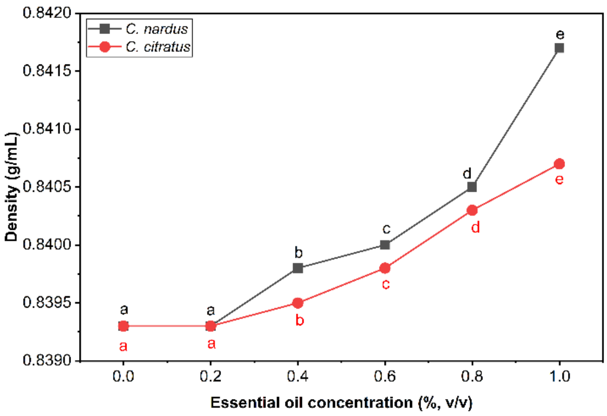

Figure 5. Effect of essential oil concentration on the density of diesel fuel blends. Different letters indicate significant differences among concentrations within each essential oil according to Fisher's LSD test (P <0.05)

3.2.2. Density

Density is a key physicochemical parameter that reflects molecular packing efficiency and the compositional characteristics of fuel systems. As shown in Figure 5, the addition of essential oils resulted in a gradual increase in density in both fuel systems. Density increased from 0.8393 g/mL for neat diesel fuel to 0.8417 g/mL for the blend containing 1.0% (v/v) *C. nardus* essential oil and to 0.8407 g/mL for the corresponding *C. citratus* blend. Two-way ANOVA revealed that essential oil type, additive concentration, and their interaction significantly affected fuel density ($p < 0.05$). Fisher's LSD test further showed that the control (0%) and 0.2% (v/v) blends were not significantly different, whereas blends containing 0.4%, 0.6%, 0.8%, and 1.0% (v/v) differed significantly, as indicated by the different letter annotations in Figure 5.

Although these differences were statistically significant, the overall increase in density was less than 0.003 g/mL, indicating only a minor practical effect on diesel fuel density. All density values remained within the diesel fuel specification range (0.815–0.870 g/mL), indicating that the addition of essential oil did not adversely affect the measured diesel fuel properties. The slight increase in density may be associated with the incorporation of relatively more polar and structurally complex molecules into the hydrocarbon matrix, thereby enhancing intermolecular cohesion compared with neat diesel fuel [31].

3.2.3. Kinematic Viscosity

Kinematic viscosity reflects the resistance to flow and is highly sensitive to intermolecular interactions and molecular size distribution. As shown in Figure 6, kinematic viscosity exhibited a slight increasing trend with increasing essential oil concentration, rising from 2.1651 to 2.1964 mm^2/s for *C. nardus* and to 2.1955 mm^2/s for *C. citratus*. Two-way ANOVA revealed that essential oil type, concentration, and their interaction significantly affected kinematic viscosity ($p < 0.05$). Fisher's LSD analysis indicated that significant differences occurred among specific concentration levels, as indicated by different letter annotations in Figure 6. Although statistically significant, the overall increase in kinematic viscosity was limited (approximately 0.03 mm^2/s), and all measured values remained within the diesel fuel specification (2.0–4.5 mm^2/s), indicating that these changes are unlikely to adversely affect fuel performance.

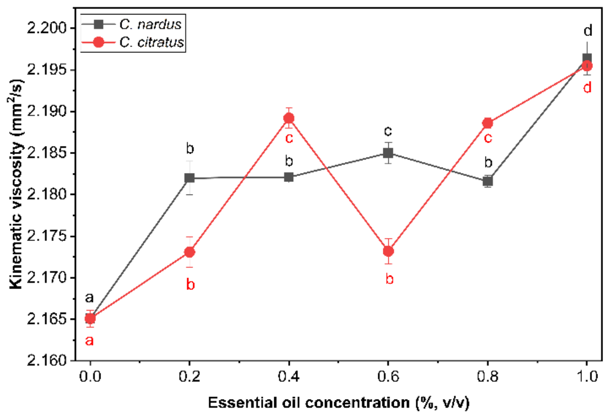

Figure 6. Effect of essential oil concentration on kinematic viscosity of diesel fuel blends. Different letters indicate significant differences among concentrations according to Fisher's LSD test ($p < 0.05$)

The observed increase may be associated with changes in intermolecular interaction within the diesel fuel matrix. Some low-molecular-weight essential oil components may act as molecular disruptors by increasing free volume and reducing intermolecular cohesion, thereby potentially decreasing kinematic viscosity. In contrast, oxygenated compounds may enhance intermolecular interactions through dipolar effects, thereby increasing resistance to flow. The resulting kinematic viscosity may therefore reflect the balance between these opposing contributions [13]. The slight increase in kinematic viscosity suggests that the interaction-enhancing effect may have outweighed the viscosity-reducing effect under the present experimental conditions.

3.2.4. Distillation Characteristics

Distillation characteristics describe the volatility distribution of fuel components and are closely related to evaporation and combustion behavior [5, 7]. As shown in Figure 7, the addition of essential oils did not significantly alter the overall shape of the distillation curves, indicating that the volatility profile remains dominated by the base diesel fuel. Minor shifts were observed in IBP, T_{10}, T_{50}, and T_{90}. The slight decrease in IBP suggests the presence of more volatile components introduced by the essential oils, whereas the increase in T_{50} and T_{90} may be associated with less volatile oxygenated constituents, such as geraniol and citronellol. These compounds require more energy to vaporize because of their stronger intermolecular interactions [32]. Nevertheless, the overall boiling range remained within diesel fuel specifications, indicating that essential oils primarily act as volatility modifiers without substantially changing the fundamental distillation behavior of the fuel.

3.2.5. Calculated Cetane Index (CCI)

The CCI is a widely used empirical parameter for estimating diesel ignition quality from density and distillation characteristics according to ASTM D4737 [5, 33]. As shown in Figure 8, increasing the essential oil concentration was associated with a gradual increase in CCI, from 45.5 to 46.3 for *C. nardus* and from 45.5 to 48.2 for *C. citratus* at 1.0% (v/v). Two-way ANOVA indicated that essential oil type, concentration, and their interaction significantly affected CCI ($p < 0.05$). Subsequent Fisher's LSD test showed that CCI generally increased with increasing essential oil concentration.

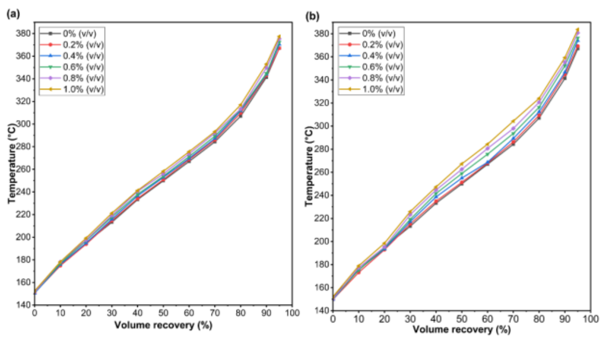

Figure 7. Distillation curves of diesel fuel blends with (a) *C. nardus* and (b) *C. citratus* essential oils

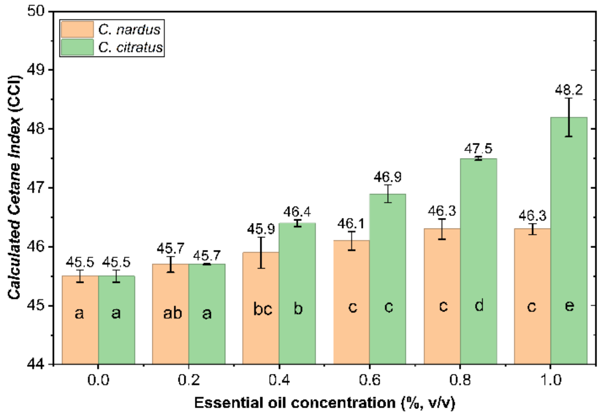

Figure 8. Effect of essential oil concentration on CCI of diesel fuel blends. Different letters indicate significant differences among concentrations according to Fisher's LSD test ($p < 0.05$)

For *C. nardus*, significant differences became apparent at concentrations of ≥0.4% (v/v), whereas *C. citratus* exhibited significant increases beginning at 0.4% (v/v), indicating a stronger response of CCI to the addition of *C. citratus* essential oil. The corresponding statistical groupings are indicated by different letter annotations in Figure 8. Therefore, the observed increase in CCI may indicate a potential improvement in ignition quality, as inferred from the ASTM D4737 calculation, and should not be interpreted as direct evidence of a shorter ignition delay or a higher cetane number.

The increase in CCI values may be associated with changes in density and distillation characteristics because these parameters are directly incorporated into the ASTM D4737 calculation. In addition, the larger increase in CCI observed for *C. citratus* coincided with its relatively higher content of oxygenated monoterpenes. The GC-MS analysis showed that oxygenated monoterpenes were the predominant chemical class in *C. citratus* (70.13%), whereas they represented only 15.64% of the identified compounds in *C. nardus* (Table 3). Geraniol and citronellol, the major oxygenated monoterpenes in *C. citratus*, contain hydroxyl (-OH) functional groups that may enhance intermolecular interactions and have been reported to promote low-temperature oxidation through the formation of oxygen-containing radical intermediates [34, 35, 36, 37]. In contrast, α-pinene, the predominant constituent of *C. nardus*, is a non-oxygenated monoterpene hydrocarbon that lacks oxygen-containing functional groups. Therefore, its direct contribution to these oxidation pathways is expected to be less pronounced. Consequently, the greater increase in CCI observed for *C. citratus* is consistent with its higher abundance of oxygenated monoterpenes.

However, no quantitative correlation or regression analysis between oxygenated compound content and CCI was performed because the chemical composition was not determined for every diesel blend concentration used in the CCI evaluation. GC-MS characterization was performed on the neat essential oils and only on the selected optimal diesel blends. Therefore, the observed relationship should be interpreted as qualitative rather than quantitative evidence.

Nevertheless, CCI remains an empirical parameter calculated from density and distillation characteristics rather than a direct measurement of ignition behavior. Furthermore, ASTM D4737 was originally developed for conventional petroleum diesel fuels, and the presence of oxygenated bioadditives may introduce deviations between the CCI and the actual cetane number. Therefore, the proposed mechanism should be regarded as a plausible interpretation rather than conclusive evidence of improved ignition performance. Confirmation through direct measurements of cetane number or ignition delay would be required in future studies. Importantly, all blends maintained CCI values above the minimum diesel specification (CCI ≥ 45), indicating compliance with the diesel fuel standard.

3.2.6. Implications for Ignition Delay

Ignition delay consists of both physical and chemical stages. The slight increases in density and kinematic viscosity observed in this study may influence spray formation and evaporation, whereas the increase in CCI suggests a potential enhancement in chemical reactivity, which may contribute to a shorter chemical ignition delay [5, 38]. However, this interpretation is inferred from the CCI values rather than direct measurements of ignition delay or cetane number.

3.2.7. Optimal Concentration Determination

The optimal concentration was selected by simultaneously considering physicochemical stability and ignition-quality enhancement. Among the blends that satisfied the diesel fuel specifications, priority was given to concentrations exhibiting relatively lower kinematic viscosity while maintaining a statistically significant improvement in CCI. The statistical criteria used for each selection step are summarized in Table 4.

For *C. nardus*, CCI showed a statistically significant increase relative to neat diesel fuel beginning at 0.4% (v/v). However, concentrations of 0.6%, 0.8%, and 1.0% (v/v) were not significantly different from one another. Among these concentrations, 0.8% (v/v) exhibited a lower kinematic viscosity than 0.6% (v/v) while maintaining a comparable CCI. Therefore, 0.8% (v/v) was selected as the optimum concentration. For *C. citratus*, CCI showed a statistically significant increase relative to neat diesel fuel beginning at 0.4% (v/v), with further significant increases observed at each subsequent concentration. However, the blend containing 0.6% (v/v) exhibited a lower kinematic viscosity than the 0.8% and 1.0% (v/v) blends while already providing a statistically significant improvement in CCI. Therefore, 0.6% (v/v) was selected as the optimum concentration by balancing ignition-quality enhancement with favorable physicochemical properties.

3.2.8. Volatile Compound Profiles of Diesel and Blended Systems

GC-MS analysis showed that the volatile compositions of neat diesel fuel and the diesel blends were generally similar (Table 5). In all samples, the major constituents were hydrocarbon compounds, including tridecane, heptadecane, nonadecane, eicosane, and heneicosane. Minor variations in the relative abundances of these compounds were observed; however, the overall hydrocarbon matrix remained largely unchanged following the addition of essential oils.

Table 4. Selection criteria for determining the optimum concentration of essential oil bioadditives

Parameter	Statistical criterion	Selected concentration	
		C. nardus	*C. citratus*
Density	Within the diesel fuel specification	All concentrations	All concentrations
Kinematic viscosity	Relatively lower kinematic viscosity while remaining comparable to neat diesel fuel	0.2%, 0.4%, 0.8% (v/v)	0.2%, 0.6% (v/v)
CCI	Statistically significant improvement relative to neat diesel fuel	≥ 0.4% (v/v)	≥ 0.4% (v/v)
Optimum concentration	Balance between kinematic viscosity and CCI	0.8% (v/v)	0.6% (v/v)

Table 5. Major hydrocarbon compounds identified by GC-MS in neat diesel fuel and diesel blends

RT (min)	Compound	Molecular formula	Neat diesel fuel (%)	+0.8% (v/v) *C. nardus* (%)	+0.6% (v/v) *C. citratus* (%)
19.315	Tridecane	$C_{13}H_{28}$	7.69	7.56	7.52
25.424	Heptadecane	$C_{17}H_{36}$	15.96	15.84	16.04
35.533	Eicosane	$C_{20}H_{42}$	6.73	ND	6.79
37.721	Nonadecane	$C_{19}H_{40}$	5.89	12.78	5.78
41.804	Heneicosane	$C_{21}H_{44}$	15.05	14.83	14.41

ND = Not detected under the GC-MS analysis conditions.

Characteristic essential-oil constituents could not be unequivocally identified due to their low concentrations relative to the diesel matrix and potential chromatographic overlap with abundant diesel hydrocarbon peaks. Therefore, the GC-MS results suggest that essential oil addition at the selected concentrations did not substantially modify the overall volatile composition of diesel fuel. This finding also suggests that the changes in physicochemical properties observed in this study were not associated with major changes in the volatile composition of the fuel, but may instead be associated with intermolecular interactions between diesel hydrocarbons and essential-oil constituents.

4. Conclusion

This study demonstrated that the chemical composition of essential oils significantly influenced the physicochemical properties and ignition quality of diesel fuel blends. Although both *C. nardus* and *C. citratus* essential oils increased the CCI. *C. citratus* produced a greater improvement in CCI, which was consistent with its higher abundance of oxygenated monoterpenes identified by GC-MS, although this relationship remains qualitative. Despite these improvements, the density, kinematic viscosity, and distillation characteristics of all blends remained within the diesel fuel specifications. Based on the combined evaluation of physicochemical properties and ignition quality, the optimum concentrations were 0.8% (v/v) for *C. nardus* and 0.6% (v/v) for *C. citratus*. These findings suggest that oxygen-rich essential oils have potential as renewable bioadditives for improving diesel ignition quality while maintaining fuel standards. However, because ignition quality was evaluated using the CCI, further studies involving direct cetane number determination, ignition delay measurements, and engine performance testing are required to validate these findings under practical engine operating conditions.

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