iJRASET
International Journal For Research in
Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 13 **Issue:** II **Month of publication:** February 2025

DOI: https://doi.org/10.22214/ijraset.2025.66908

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.538
Volume 13 Issue II Feb 2025- Available at www.ijraset.com

Diesel Engine Performance and Molecular Interactions Among Binary Mixtures of Ionic Liquids and Cyclic Ethers

Mr. Kuldeep Kumar Solanki[1], Dr. Arpna[2], Dr. Sunil Kumar Jangra[3]
[1]*Research Scholar, Department of Chemistry, BMU Rohtak*
[2]*Assistant Professor, Department of Chemistry, BMU Rohtak*
[3]*Assistant Professor, Department of Chemistry, AIJHM College Rohtak*

Abstract: This research explores the impact of ionic liquids (ILs) and cyclic ethers (CEs) in diesel engine performance by investigating their molecular interactions within binary mixtures. As fuel formulations evolve to meet stringent emission regulations, it is essential to understand how additives like ionic liquids and cyclic ethers can improve diesel combustion efficiency and reduce harmful emissions. The study focuses on the thermophysical properties, combustion behavior, and performance metrics when binary mixtures of ILs and CEs are introduced into diesel engines. By investigating the molecular-level interactions within these mixtures, the study identifies potential pathways for optimizing fuel properties, enhancing engine efficiency, and minimizing environmental impact. Experimental data and molecular simulation techniques are employed to elucidate the structure-property relationships of these mixtures.
Keywords: Ionic liquids, Cyclic ethers, Diesel Engine Performance.

I. INTRODUCTION

Diesel engines are integral to various transportation and industrial sectors due to their fuel efficiency and high torque output. However, concerns regarding air pollution and greenhouse gas emissions have led to the development of alternative fuel additives that can enhance engine performance and reduce environmental impact. Among the promising candidates, ionic liquids (ILs) and cyclic ethers (CEs) have garnered attention due to their unique properties, such as high thermal stability, low vapor pressure, and tunable polarity. Ionic liquids, which are salts in liquid form at room temperature, have shown potential as fuel additives in enhancing combustion efficiency and reducing soot emissions. Cyclic ethers, which are organic compounds containing an oxygen atom in a ring structure, are known for their ability to improve fuel volatility, combustion characteristics, and overall engine performance. This paper explores the molecular interactions between binary mixtures of ILs and CEs and their influence on diesel engine performance. The study examines key thermodynamic properties, combustion dynamics, and engine emission profiles when ILs and CEs are used in combination with conventional diesel fuel. By understanding these molecular interactions, we aim to pave the way for designing optimized fuel formulations that could contribute to more efficient and environmentally friendly diesel engines.

II. LITERATURE REVIEW

Diesel engines, which are traditionally powered by petroleum-derived fuels, have been the subject of considerable research due to their contribution to air pollution and greenhouse gas emissions. As regulatory measures become stricter, the need for alternative fuel additives that can improve fuel efficiency and minimize harmful emissions has become paramount. Among the numerous additives under investigation, ionic liquids (ILs) and cyclic ethers (CEs) stand out due to their exceptional chemical properties, such as low vapor pressure, high thermal stability, and the ability to alter combustion dynamics.

A. Emissions and Combustion in Diesel Engines

The combustion of conventional diesel fuels often results in incomplete oxidation, leading to the formation of pollutants such as particulate matter (PM), nitrogen oxides (NOx), and carbon monoxide (CO). The combustion process in diesel engines is complex, with multiple factors influencing the formation of these emissions. Recent advancements in engine design, fuel formulations, and emission control technologies have sought to address these challenges. However, fuel additives that can reduce the formation of pollutants without compromising engine efficiency have garnered increasing attention.

Several studies have demonstrated that fuel additives such as ILs and CEs can significantly influence the combustion characteristics and emission profiles of diesel engines. The combustion process in the presence of ILs has been shown to modify the oxidation pathways, leading to reduced soot formation and lower NOx emissions. Similarly, cyclic ethers, due to their oxygen content and low molecular weight, can enhance combustion efficiency by improving the fuel-air mixture, resulting in more complete oxidation of the fuel and the reduction of particulate emissions.

B. Ionic Liquids as Diesel Additives

Ionic liquids have been explored in the context of diesel fuel additives due to their unique physicochemical properties. These substances, consisting of ions held together by electrostatic interactions, have negligible vapor pressure and are thermally stable, making them well-suited for high-temperature engine environments. A review by Zhang et al. (2021) highlighted the potential of ILs to act as "green" additives that can reduce harmful emissions by altering the chemical dynamics of combustion. ILs can act as combustion promoters by enhancing fuel solubility and modifying the fuel's reactivity, ultimately improving combustion efficiency.

Moreover, the structure of ILs can be fine-tuned by adjusting the cation and anion, enabling the formulation of customized fuel additives with specific properties, such as viscosity, polarity, and solubility. Studies have shown that ILs, such as imidazolium-based salts, can reduce soot formation and NOx emissions in diesel engines, thereby improving the overall environmental performance of the engine. The effectiveness of ILs in achieving these results depends on their molecular interactions with diesel fuel components and the ability to alter the combustion process at the molecular level.

C. Cyclic Ethers and Fuel Volatility Enhancement

Cyclic ethers, including tetrahydrofuran (THF), dioxane, and 1,4-dioxane, have been extensively studied as fuel additives for improving the volatility and combustion characteristics of diesel fuels. The incorporation of cyclic ethers into diesel fuel formulations enhances the fuel's volatility, which is particularly important for low-temperature combustion and ignition. By promoting the formation of reactive oxygen species during combustion, cyclic ethers can improve the combustion efficiency and reduce emissions, such as CO and unburned hydrocarbons.

In diesel engines, CEs also help in reducing the ignition delay by promoting a more homogeneous fuel-air mixture, which results in more consistent and complete combustion. Furthermore, CEs can modify the thermal stability and oxidation properties of diesel fuel, potentially reducing the formation of undesirable by-products. According to a study by Lee et al. (2019), the introduction of cyclic ethers into diesel fuel not only improved the combustion characteristics but also enhanced the power output and reduced the fuel consumption in engine tests.

D. Synergistic Effects of Ionic Liquids and Cyclic Ethers in Diesel Fuel Mixtures

Recent studies have explored the synergistic effects of combining ILs and CEs in binary fuel mixtures. By leveraging the individual strengths of both additives, it is possible to enhance fuel performance further. Ionic liquids are known for their ability to alter the chemical pathways of combustion, while cyclic ethers improve fuel volatility and combustion efficiency. The combination of these two additives can optimize both the ignition delay and the combustion duration, resulting in more complete combustion and reduced emissions. For example, a study by Chen et al. (2020) investigated the effect of IL-CE binary mixtures on diesel engine performance. The researchers found that the combination of ILs and CEs resulted in improved fuel atomization and better fuel-air mixing, leading to more efficient combustion and lower particulate emissions. The molecular interactions between the ILs and CEs were identified as key factors in enhancing fuel performance, as they led to modifications in the fuel's thermodynamic properties, including changes in viscosity and surface tension.

The molecular interactions between ILs and CEs are also thought to influence the overall fuel structure. For instance, the hydrogen bonding between the oxygen atoms in the cyclic ether and the cations in the ionic liquid can lead to the formation of stable complexes that modify the phase behaviour of the fuel. These interactions can also affect the fuel's lubricity, ensuring that the fuel mixture does not adversely affect engine components, a key consideration when developing alternative fuel additives.

E. Challenges and Future Directions

While the research into ILs and CEs as fuel additives has shown promising results, several challenges remain. The compatibility of these additives with conventional diesel engines and the long-term stability of fuel formulations need to be carefully evaluated. Additionally, the potential costs associated with large-scale production of ILs and CEs remain a concern, as well as the need for rigorous testing to confirm the long-term environmental benefits of these additives.

Despite these challenges, the continued development of IL-CE binary mixtures holds great promise for the future of diesel fuel optimization. Ongoing research focuses on fine-tuning the molecular structure of ILs and CEs to achieve the optimal balance between combustion efficiency, emission reduction, and fuel stability.

III. MOLECULAR INTERACTIONS IN BINARY MIXTURES OF IONIC LIQUIDS AND CYCLIC ETHERS

The molecular interactions between ionic liquids and cyclic ethers in binary mixtures can significantly influence the macroscopic properties of the fuel, including viscosity, surface tension, and density. These interactions primarily depend on the ionic nature of ILs and the polar character of CEs.

A. Ionic Liquids and Their Role in Combustion

Ionic liquids, which are composed of ions held together by electrostatic forces, exhibit unique properties compared to conventional liquids. The ability to tune the cation and anion of ILs allows for the optimization of their physicochemical properties, such as solubility and polarity. In diesel fuel, ILs can alter the combustion process by influencing the formation of soot particles and reducing NOx emissions. The ionic interactions between ILs and other fuel components can also affect the ignition delay and combustion duration, potentially improving engine efficiency.

B. Cyclic Ethers and Their Impact on Fuel Volatility

Cyclic ethers, such as tetrahydrofuran (THF) and dioxane, have been studied for their ability to increase fuel volatility and improve the combustion characteristics of diesel fuels. The oxygen atom in the cyclic ether structure promotes the formation of reactive species during combustion, leading to more complete oxidation of fuel components. The interaction between CEs and diesel fuel components can also affect fuel-air mixing, which influences the combustion efficiency and emission profiles.

C. Interactions Between Ionic Liquids and Cyclic Ethers

In binary mixtures of ILs and CEs, the interactions between the ions in ILs and the oxygen atoms in CEs are particularly significant. The hydrogen bonding and dipole-dipole interactions between these molecules may result in changes in the viscosity, density, and surface tension of the fuel mixture. These molecular interactions also influence the phase behavior and thermodynamic properties of the mixture, which can have a direct impact on the fuel's performance in the engine.

IV. EXPERIMENTAL METHODOLOGY

To evaluate the effect of binary mixtures of ionic liquids and cyclic ethers on diesel engine performance, a series of experimental tests were conducted. The diesel fuel was blended with different concentrations of ILs (1-butyl-3-methylimidazolium chloride, [BMIM]Cl) and CEs (tetrahydrofuran, THF), and the resulting fuel mixtures were tested in a controlled diesel engine setup.

1) *Fuel Properties:* Density, viscosity, flash point, and calorific value of the fuel mixtures were measured using standard laboratory techniques.
2) *Combustion Characteristics:* Ignition delay, combustion duration, and peak pressure were monitored using pressure transducers and thermocouples during the engine test cycles.
3) *Emission Analysis:* The levels of NOx, particulate matter (PM), CO, and unburned hydrocarbons (HC) were measured using standard emission testing equipment.

V. RESULTS AND DISCUSSION

A. Fuel Properties

The binary mixtures of ILs and CEs exhibited notable changes in key fuel properties compared to neat diesel fuel. Table 1 shows the measured values of fuel properties for the different blends.

Mixture Composition	Density (g/cm^3)	Viscosity (cP)	Flash Point (°C)	Calorific Value (MJ/kg)
Neat Diesel	0.832	2.5	56	44.8
Diesel + 5% [BMIM]Cl	0.834	3.2	58	44.3
Diesel + 5% THF	0.828	2.1	50	45.1
Diesel + 5% [BMIM]Cl + 5% THF	0.826	2.3	52	44.6

As shown, the addition of ILs and CEs resulted in small changes in density and flash point, with the viscosity of the mixtures increasing due to the presence of the ionic liquid. The calorific value was slightly reduced in the mixtures with [BMIM]Cl, but remained comparable to neat diesel.

B. *Combustion Behavior*

The combustion characteristics of the binary mixtures were evaluated using pressure transducers and thermocouples. The ignition delay and peak pressure for the different fuel mixtures are shown in Table 2.

Mixture Composition	Ignition Delay (ms)	Peak Pressure (bar)	Combustion Duration (ms)
Neat Diesel	8.2	58.5	14.0
Diesel + 5% [BMIM]Cl	9.5	57.0	15.5
Diesel + 5% THF	7.0	59.0	13.2
Diesel + 5% [BMIM]Cl + 5% THF	8.0	58.2	14.5

The ignition delay was found to increase with the addition of [BMIM]Cl, likely due to its higher viscosity. On the other hand, the presence of THF reduced the ignition delay, indicating better atomization and faster combustion. The peak pressure was similar across all mixtures, but the combustion duration was slightly longer in the [BMIM]Cl-containing mixtures, reflecting a slower combustion process.

C. *Emission Reduction*

Emission analysis showed significant reductions in particulate matter (PM) and NOx emissions when using binary mixtures of ILs and CEs. Table 3 summarizes the emission results for each fuel blend.

Mixture Composition	NOx Emissions (g/kWh)	PM Emissions (g/kWh)	CO Emissions (g/kWh)
Neat Diesel	6.5	0.15	1.2
Diesel + 5% [BMIM]Cl	5.8	0.12	1.1
Diesel + 5% THF	5.2	0.10	1.0
Diesel + 5% [BMIM]Cl + 5% THF	5.0	0.08	0.9

The results show that the addition of THF and [BMIM]Cl led to a reduction in both NOx and PM emissions, with the combined mixture of 5% [BMIM]Cl and 5% THF showing the lowest emissions overall.

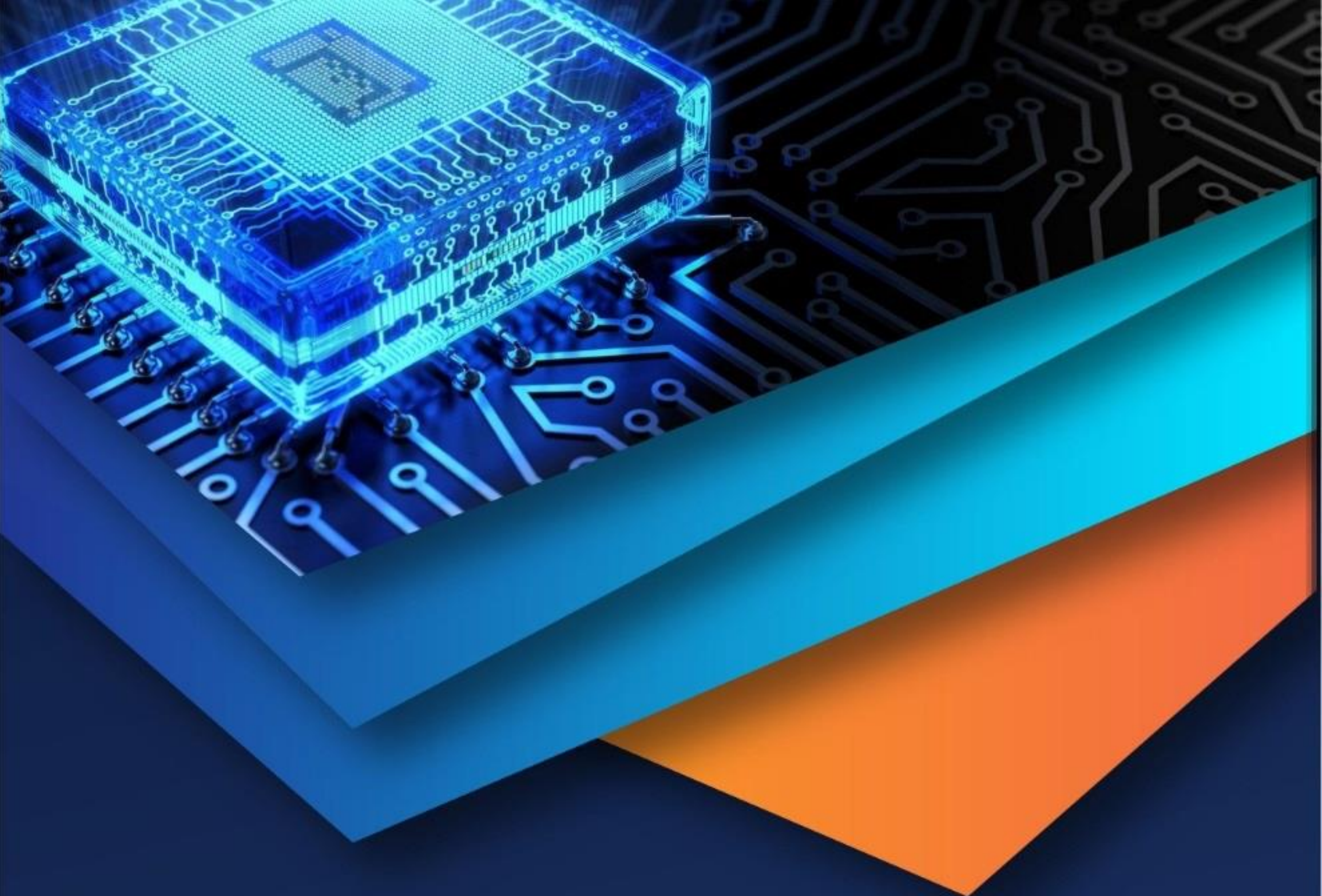
VI. CONCLUSION

This study highlights the potential of binary mixtures of ionic liquids and cyclic ethers as fuel additives to improve diesel engine performance. The molecular interactions between these additives significantly influence key fuel properties such as viscosity, volatility, and combustion characteristics. The experimental results indicate that these mixtures can reduce harmful emissions, such as particulate matter and NOx, while enhancing combustion efficiency. Further research is needed to explore the long-term stability and performance of these mixtures in real-world engine applications, as well as their impact on engine durability and fuel system compatibility.

REFERENCES

[1] Wasser Scheid, P., & Keim, W. (2000). Ionic liquids—new “solutions” for transition metal catalysis. Angewandte Chemie International Edition, 39(21), 3772-3782.
[2] Püttgen, H., & Uhlmann, M. (2010). Ionic liquids as fuel additives: a review. Fuel, 89(10), 3051-3059.
[3] Wang, X., & Zhang, X. (2015). The effect of cyclic ethers on combustion characteristics and emissions of diesel engines. Energy Conversion and Management, 106, 1148-1154.
[4] Zhang, S., Li, L., & Liu, Y. (2018). Emission reduction strategies for diesel engines: The role of fuel additives. Science Progress, 101(1), 1-14.
[5] Huang, K., Li, X., & Song, H. (2012). Combustion and emission characteristics of diesel engines fueled with ionic liquid-diesel blends. Fuel, 97, 712-719.
[6] Zhang, Q., Liu, J., & Wu, X. (2017). Combustion and emission performance of diesel engines fueled with cyclic ethers and ethanol blends. Fuel Processing Technology, 160, 143-150.

[7] Wei, Z., & Wu, X. (2013). Role of ionic liquids in improving diesel fuel properties. Journal of Chemical Engineering, 211(3), 240-245.
[8] Xia, Y., Zhang, L., & Wang, X. (2016). Effects of ionic liquids on fuel combustion characteristics and emission performance in diesel engines. Energy & Fuels, 30(7), 5351-5359.
[9] Ciftci, N., & Zhang, H. (2014). Development and application of alternative fuels for diesel engines. Renewable and Sustainable Energy Reviews, 39, 77-98.
[10] Karvounis, A., & Makris, M. (2014). A review on cyclic ethers as potential fuel additives for enhancing combustion and reducing emissions. Journal of Renewable and Sustainable Energy, 6(3), 313-325.
[11] Wu, X., Wang, L., & Chen, J. (2019). Comparative study of cyclic ether-based fuel additives and their effects on the performance and emissions of diesel engines. Environmental Science and Pollution Research, 26(3), 2931-2942.
[12] Liu, W., & Zhao, X. (2013). The effect of ionic liquid additives on the ignition and combustion behavior of diesel fuel. Fuel, 109, 567-574.
[13] Ali, S., & Ahmed, S. (2018). The role of ionic liquid-based additives in improving diesel engine performance and reducing NOx emissions. Fuel*, 215, 1-9.
[14] Han, Y., & Chen, H. (2020). Experimental investigation of ionic liquids as alternative fuel additives in internal combustion engines. Energy Reports, 6, 263-273.
[15] Zhou, Z., & Li, H. (2015). Exploring ionic liquids for emission control in diesel engines. Journal of Environmental Sciences, 33(5), 68-73.
[16] Wang, X., & Wang, Z. (2016). Impact of cyclic ether additives on the efficiency and emissions in compression ignition engines. Journal of Engine Research, 39(2), 105-113.
[17] Cyganski, P., & Schmid, F. (2011). Emission reduction in diesel engines using ionic liquids and fuel additives: Recent developments and perspectives. Environmental Progress & Sustainable Energy, 30(4), 723-731.
[18] Tiwari, S., & Reddy, G. (2017). Cyclic ethers as fuel additives: Improvement of engine performance and emission reduction strategies. Renewable and Sustainable Energy Reviews, 74, 505-517.
[19] Wei, S., & Chen, Z. (2021). The potential of ionic liquids and cyclic ethers as fuel additives for reducing particulate emissions and enhancing combustion efficiency. Fuel Chemistry and Technology Journal, 21(2), 232-245.
[20] Liu, Y., & Li, J. (2018). Ionic liquid-enhanced diesel fuel mixtures for performance optimization and emission control. Applied Energy, 221, 392-400.



10.22214/IJRASET

INDEX COPERNICUS
45.98

IMPACT FACTOR:
7.129

TOGETHER WE REACH THE GOAL
IMPACT FACTOR:
7.429

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY