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A study on the characteristics of ^{1}H NMR spectra and evaluation of the sensitivity of an electromagnetic induction system to differences in the research octane number of petroleum fuels

Rohmah Insyirah Handayani[1], Bambang Murdaka Eka Jati[2], Eka Sulistya[3]

[1,2,3]Department of Physics, Universitas Gadjah Mada, Yogyakarta, Indonesia

[1] rohmahinsyirah@mail.ugm.ac.id, [2] b_murdaka@ugm.ac.id, [3] sulistya@ugm.ac.id

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Abstract: The Research Octane Number (RON) is a key quality parameter of gasoline that reflects the molecular structural characteristics of hydrocarbons; however, its conventional determination relies on standardized engine testing, which is impractical for rapid laboratory analysis. This study aims to analyze the characteristics of 1H NMR spectra of gasoline with different RON values and to evaluate the potential of alternative approaches based on electromagnetic induction and capacitive methods as discriminative parameters for RON. The methodology includes 1H NMR spectral analysis using region-based integration of chemical shifts without individual compound identification, as well as evaluation of the response of mutual induction systems and RC and RLC capacitive circuits to various gasoline samples. The results show that 1H NMR spectra exhibit clear differences in the distribution of aliphatic and aromatic signals among gasoline samples with different RON values, whereas the electromagnetic induction system does not demonstrate sufficient sensitivity due to the non-magnetic nature of gasoline. The capacitive approach is capable of detecting media with large permittivity contrast but is not yet sufficiently sensitive to discriminate subtle variations among gasoline samples. This study provides a methodological basis for the application of 1H NMR in the molecular structural characterization of gasoline and a critical evaluation of the limitations of sensor-based approaches relying on electromagnetic responses.

Keyword : Research Octane Number; 1H NMR; gasoline; electromagnetic induction; capacitive sensor

1. Introduction

The Research Octane Number (RON) is a primary quality parameter of gasoline that represents the fuel's resistance to knocking phenomena in spark-ignition engines. Fundamentally, the RON value is determined by the molecular structure of the constituent hydrocarbons, particularly the degree of chain branching, aromatic content, and the distribution of aliphatic and olefinic groups (Pavia et.al, 20; Rahat et.al, 2023) Branched and aromatic hydrocarbons generally exhibit higher RON values than straight-chain

hydrocarbons; therefore, RON is essentially a chemical–structural parameter rather than merely a macroscopic physical property.

The standard method for determining RON still relies on Cooperative Fuel Research (CFR) engine testing in accordance with ASTM standards, which is complex, costly, and impractical for rapid laboratory analysis or the development of physics-based sensors. These limitations have motivated the exploration of alternative methods that are non-destructive, rapid, and capable of accurately representing fuel characteristics. However, a major challenge of such alternative approaches lies in the compatibility between the underlying physical principles of the method and the molecular properties that govern the RON value.

Nuclear Magnetic Resonance (NMR) spectroscopy, particularly ^1H NMR, is an analytical technique capable of directly and quantitatively mapping the chemical environments of protons in complex hydrocarbon mixtures (Diehl, B., & Randel, G.,2027)(Jenie et.al.,2017) The 1H NMR spectrum of gasoline exhibits characteristic signal distributions in the aliphatic, olefinic, and aromatic regions, which can serve as compositional fingerprints of the fuel. Several studies have demonstrated that 1H NMR spectra combined with chemometric analyses such as Principal Component Analysis (PCA) and Partial Least Squares (PLS) can predict octane numbers with high accuracy, approaching that of standard methods (Al Ibrahim, E., & Farooq, A. 2020)(Pinto et al., 2020).

Nevertheless, chemometric-based predictive approaches have inherent conceptual limitations. Statistical models are highly dependent on the quality and representativeness of the training data and often function as black boxes, such that the physical relationship between changes in spectral characteristics and RON values is not always explicitly explained. Moreover, generalization of the models to different gasoline types or RON ranges requires further validation (Al Ibrahim, E., & Farooq, A. 2020). Therefore, the analysis of ^{1}H NMR spectra based on region-wise chemical shift integration, without direct predictive claims, represents a relevant alternative approach for examining differences in fuel molecular structure at a more fundamental level.

In addition to spectroscopic methods, various sensor approaches based on electromagnetic responses have been developed for fuel characterization, particularly for fuel type classification and adulteration detection. Resonator- and microwave-based sensors have been reported to distinguish fuels based on changes in the dielectric properties of the medium (Rahad et,al., 2023)(Wu et.al., 2025). However, the application of electromagnetic induction approaches to differentiate RON values faces fundamental limitations. Gasoline is a non-magnetic liquid with a relative magnetic permeability very close to unity; consequently, variations in hydrocarbon molecular structure that influence RON do not produce significant changes in magnetic flux (Pavia et.al, 2015). As a result, the response of inductive systems is more strongly influenced by geometric factors and circuit configuration than by differences in RON values.

Based on these considerations, this study aims to analyze the characteristics of 1H NMR spectra of gasoline with different RON values using a region-based chemical shift integration approach, without individual compound identification or advanced

chemometric modeling. In addition, this study experimentally evaluates the sensitivity and limitations of mutual electromagnetic induction approaches and RC and RLC capacitive systems in the context of RON determination. This work contributes a comparative evaluation grounded in physical principles regarding the suitability of each method for probing the chemical parameters represented by RON, and it further emphasizes the relevance of ^{1}H NMR spectroscopy as a primary approach for the structural characterization of fuels.

2. Methodology

2.1. Materials and Samples

The samples used in this study consisted of a solvent that also served as a reference standard, and the fuel samples themselves. The solvent and reference standard employed was CDCl3-D1 (deuterated chloroform) with the addition of 0.03% tetramethylsilane (TMS). This solvent was selected due to its ability to dissolve hydrocarbon compounds and to provide high-resolution ^{1}H NMR spectra. The residual proton signal of the CDCl3 solvent appears at $\delta \approx 7.26$ ppm and serves as a secondary internal reference for chemical shift calibration, while TMS is used as the primary reference at 0 ppm for absolute chemical shift scaling.

The primary test samples consisted of petroleum fuels in the categories of gasoline and diesel, obtained from public fuel stations in Indonesia. The gasoline samples covered RON values of 90, 92, and 98, while diesel samples were characterized by Cetane Numbers (CN) of 51 and 53. All samples were analyzed in their original form without any additional chemical treatment in order to preserve a molecular composition representative of real market conditions.

2.2. ^{1}H NMR Spectral Data Acquisition

^{1}H NMR spectral measurements were performed using a high-resolution NMR instrument with a fixed magnetic field. The fuel samples were dissolved in the appropriate deuterated solvent and placed in standard NMR tubes. Data acquisition was carried out using a single radiofrequency pulse experiment to obtain the free induction decay (FID) signal. The FID data were subsequently processed by Fourier transformation to generate ^{1}H NMR spectra expressed in chemical shift units (ppm). Chemical shift calibration was performed with respect to the appropriate internal reference. Spectral resolution was maintained consistently across all samples to ensure comparability of the results.

2.3. ^{1}H NMR Spectral Analysis

The ^{1}H NMR spectra were analyzed using a region-based chemical shift integration approach. The spectra were divided into several main regions representing aliphatic, olefinic, and aromatic proton environments. Integration was performed for each region to obtain the relative distribution of signal intensities as a quantitative representation of proton environments. This analysis did not involve the identification or quantification of

individual compounds, nor did it employ chemometric approaches or predictive models for RON estimation.

2.4. Mutual Electromagnetic Induction System

The electromagnetic induction response was evaluated using a primary–secondary coil system configured in a mutual induction arrangement. The primary coil was excited with an alternating current signal from a function generator at a specified frequency, while the induced voltage in the secondary coil was measured using a digital oscilloscope. Fuel samples were placed in a non-conductive container and positioned between the coils according to the measurement configuration. Measurements were conducted under identical excitation conditions for all samples to assess the sensitivity of the system to variations in fuel type and RON value.

2.5. Capacitive System Based on RC and RLC Circuits

As an alternative approach, experiments were conducted using capacitive systems based on RC and RLC circuits. The test capacitor was immersed in different media, namely air, water, and fuel, to evaluate the system response to changes in the medium's permittivity. The circuit response was monitored through variations in the peak-to-peak voltage observed on an oscilloscope. The circuit configuration and excitation parameters were kept constant throughout the measurements to ensure that any observed response changes originated from differences in the test media.

2.6. Evaluation Approach and Methodological Limitations

The evaluation was performed comparatively by examining the capability of each method to distinguish variations in fuel types based on the measured responses. This study is exploratory in nature and does not include calibration against industrial standard instruments such as the CFR engine. In addition, the influence of external factors such as temperature and ambient humidity variations was not considered as an independent variable in the analysis.

3. Results and Discussion

3.1. Characteristics of ^{1}H NMR Spectra of Fuels with Different RON Values

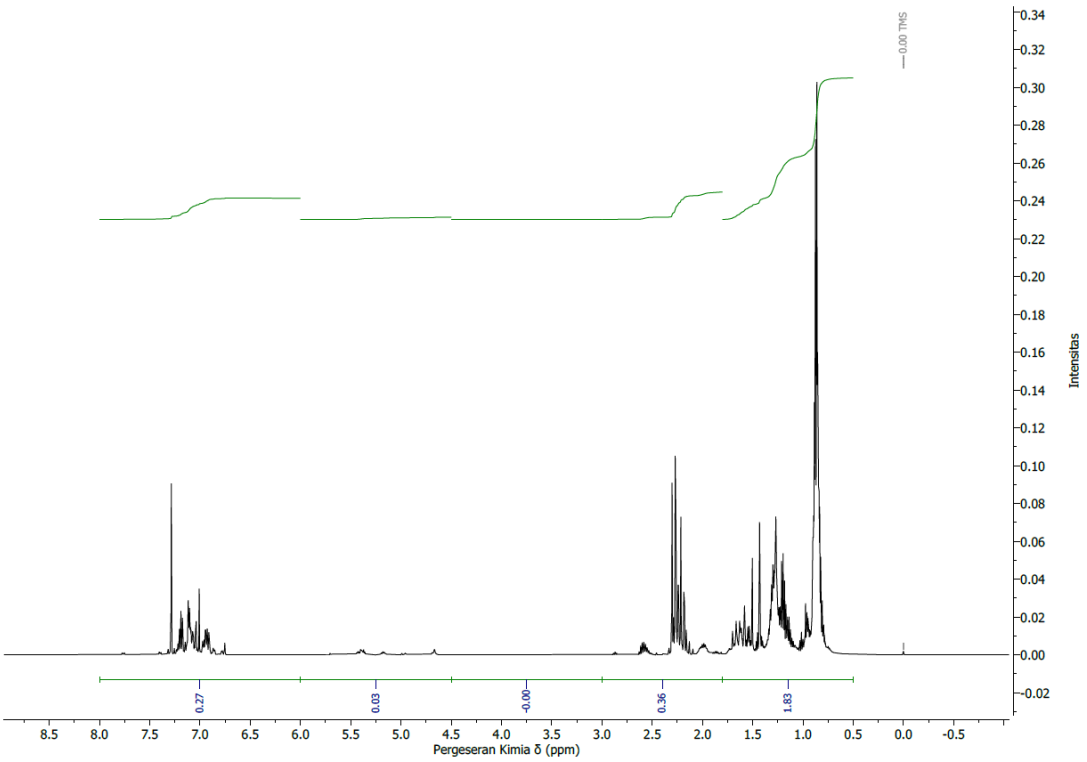
The ^{1}H NMR spectra of fuel samples with different RON values exhibit generally similar patterns, with dominant signals in the aliphatic region (0.5–3.0 ppm) and smaller contributions in the olefinic (4.5–6.0 ppm) and aromatic (6.0–8.0 ppm) regions, as shown in Figure 1. Although no significant peak shifts are observed among the samples, region-based integration analysis reveals differences in the relative distribution of signal intensities across the chemical shift regions, as presented in Table 1.

Based on Table 1, samples with higher RON values (RON 98) show an increased contribution of signals in the 3.0–4.5 ppm region and in the olefinic region (4.5–6.0 ppm) compared with RON 90 and 92. This trend indicates the presence of branched aliphatic structures and unsaturated compounds. Meanwhile, the contribution of the aromatic

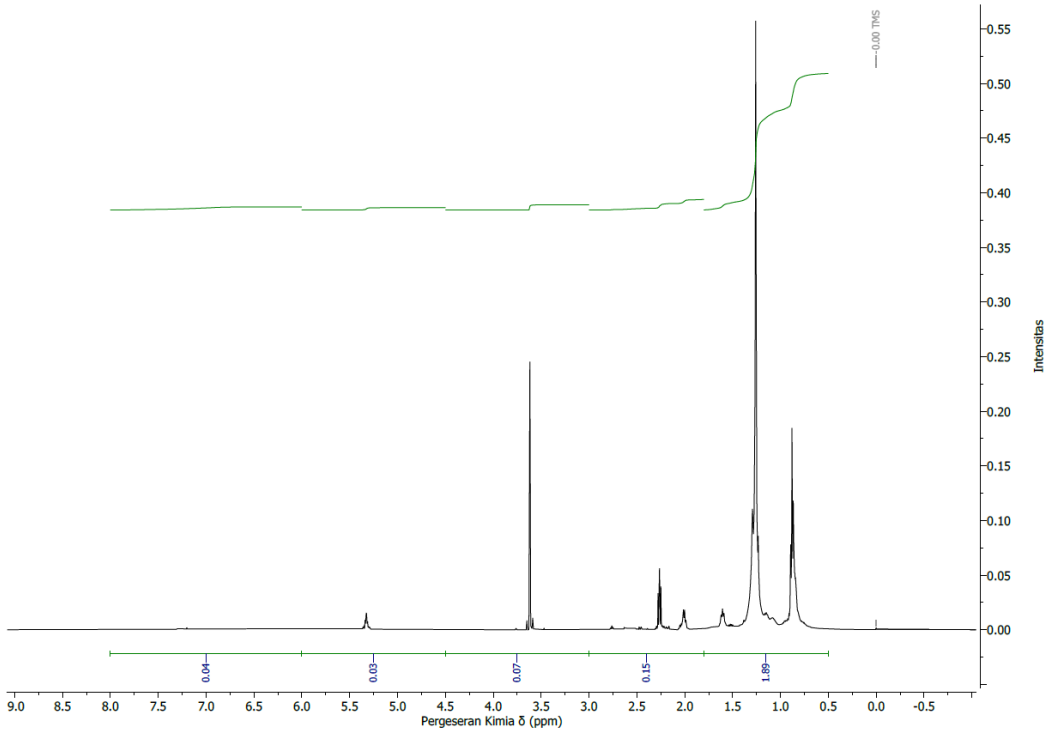
region (6.0–8.0 ppm) exhibits a decreasing trend with increasing RON, suggesting that, within the range of samples examined, the increase in RON is not solely mediated by aromatic content but is also influenced by the presence of branched and olefinic structures. In contrast, diesel samples (CN 51 and CN 53) are dominated by straight-chain aliphatic signals (>86%), with very low aromatic and olefinic contributions, consistent with the characteristics of saturated hydrocarbons in diesel fuel.

Table 1. Relative distribution of hydrocarbon protons obtained from ^{1}H NMR spectral integration for different fuel classes

	0.5-1.8 ppm (Aliphatic) (%)	1.8-3.0 ppm (%)	3.0-4.5 ppm (%)	4.5-6.0 ppm (Olefinic) (%)	6.0-8.0 ppm (Aromatic) (%)
RON 90	73.49	14.46	0	1.20	10.84
RON 92	72.91	13.94	1.59	1.59	9.96
RON 98	75.00	11.46	3.12	3.12	7.29
CN 51	86.70	6.88	3.21	1.38	1.83
CN 53	96.26	3.21	0	0	0.53



RON 90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Intensitas
Pergeseran Kimia δ (ppm)
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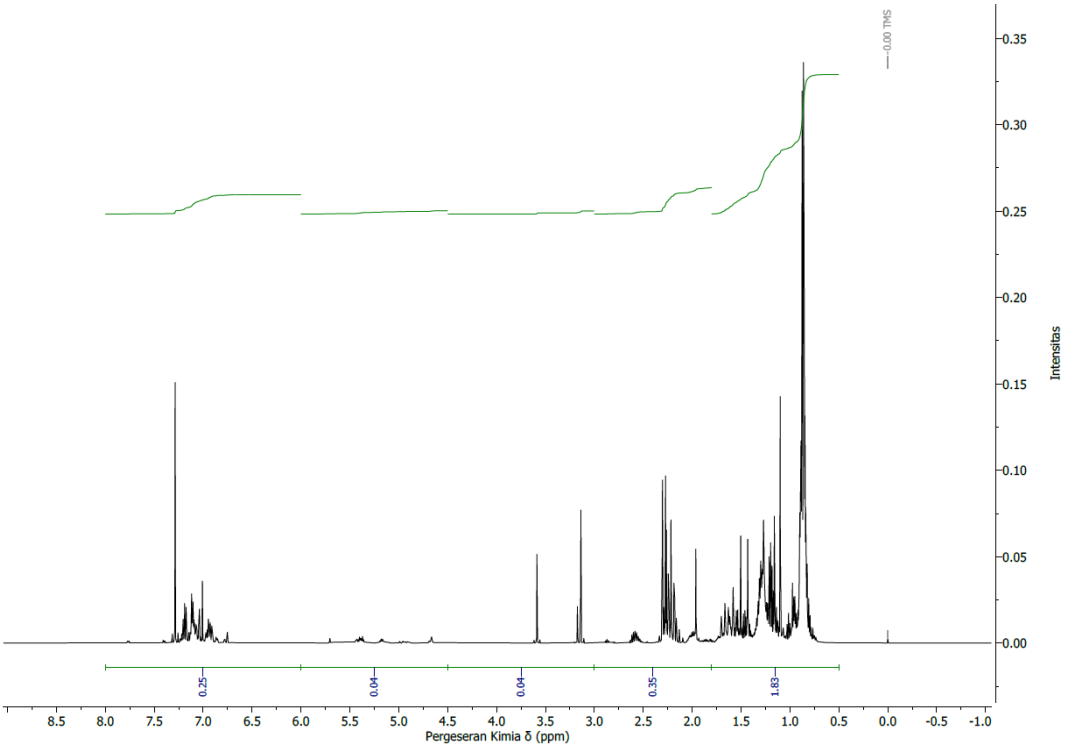
0.03
0.07
0.15
1.89

CN51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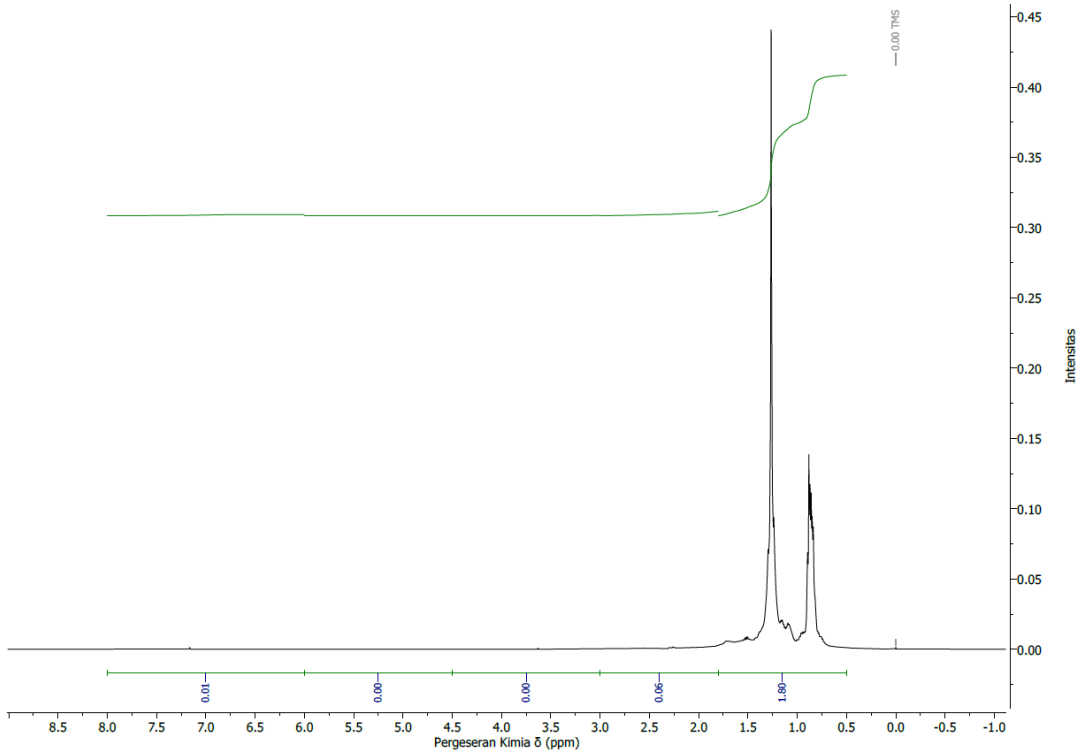
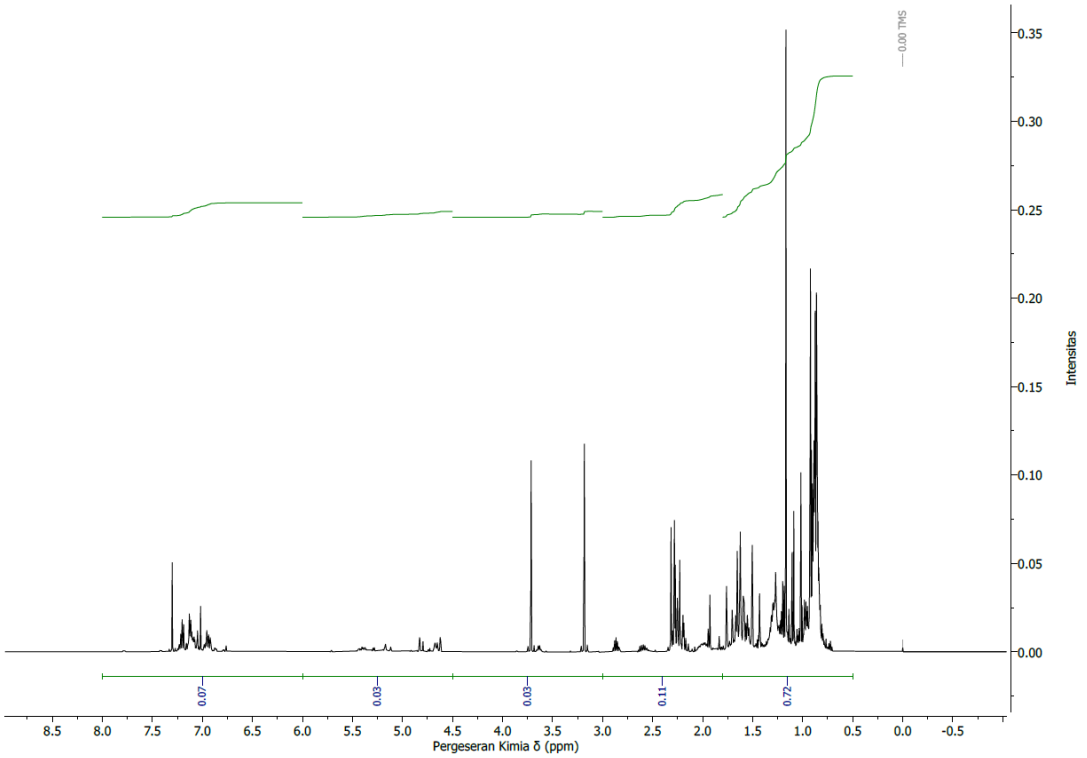
0.04
0.04
0.35
1.83

RON 92



CN53



RON 98

Figure 1. Representative ^{1}H NMR spectra of fuel samples with varying RON and CN values

These results are consistent with fundamental fuel chemistry principles, in which branched and unsaturated structures enhance resistance to auto-ignition. Accordingly,

although gasoline ^{1}H NMR spectra are complex and highly overlapping, the region-based integration approach is capable of revealing structural differences that are relevant to RON values without the need to identify individual compounds.

3.2. Physical Interpretation of the NMR Region-Based Integration Approach

The chemical shift region integration approach provides a quantitative representation of proton environments without requiring the identification of individual compounds. This is important because gasoline is a multicomponent mixture containing hundreds of compounds, making single-compound–based analytical approaches impractical. Unlike chemometric approaches, this method does not aim to generate a predictive model for RON values, but rather to examine the direct relationship between the distribution of proton environments and trends in RON.

However, it should be emphasized that differences in intensity distribution among regions are not necessarily linear with respect to increases in RON. This indicates that RON is determined by a complex combination of multiple molecular structures rather than by a single spectral parameter. Accordingly, these results reinforce the role of 1H NMR as a structural analysis tool rather than as a direct substitute for standard RON determination methods.

3.3. Response of the Mutual Electromagnetic Induction System

Measurements using the mutual electromagnetic induction system indicate that the induced voltage measured at the secondary coil does not exhibit significant variation among fuel samples with different RON values. The observed response variations fall within the range of measurement fluctuations and do not display a consistent pattern with respect to RON.

These results confirm the fundamental limitations of inductive approaches for RON characterization. Because gasoline is a non-magnetic medium with a relative magnetic permeability close to unity, variations in hydrocarbon molecular structure do not produce detectable changes in magnetic flux. In other words, the insensitivity of the induction system to RON variations is not merely due to experimental limitations, but rather to a mismatch between the physical principles of the method and the chemical parameters being probed.

3.4. Response of RC and RLC Capacitive Systems to Test Media

Testing of the capacitive systems shows clear response differences when the capacitor is immersed in air, water, and fuel. These differences reflect the large contrast in relative permittivity among the media. However, when comparing fuel samples with different RON values, the response changes in both RC and RLC circuits are very small and do not exhibit consistent trends.

This indicates that differences in relative permittivity among gasoline types lie within a narrow range and are below the sensitivity limit of simple capacitive systems. Furthermore, the contribution of parasitic capacitance and measurement uncertainty

further reduces the system's ability to detect such small variations. Therefore, although capacitive approaches are theoretically more relevant for non-magnetic liquids than inductive approaches, simple RC- and RLC-based implementations are not yet sufficient to reliably discriminate RON values.

3.5. Comparison among Methods

Overall, ^{1}H NMR spectroscopy demonstrates the most direct sensitivity to differences in hydrocarbon molecular structures that underlie RON values. In contrast, electromagnetic induction and capacitive approaches probe macroscopic physical properties of the medium that are only indirectly correlated, or even uncorrelated, with the chemical parameters that determine RON. These findings emphasize that the selection of a method for RON characterization must consider the compatibility between the physical principles of the method and the molecular properties of the fuel.

4. Conclusion

This study demonstrates that a 1H NMR spectroscopic approach based on chemical shift region integration is capable of revealing differences in proton environment distributions in fuels with different RON values, reflecting variations in the underlying hydrocarbon molecular structures. This approach is effective as a structural analysis tool for distinguishing fuel characteristics without requiring individual compound identification or predictive modeling of RON values.

In contrast, the mutual electromagnetic induction approach does not exhibit sufficient sensitivity to variations in RON, a limitation that is fundamentally attributable to the non-magnetic nature of gasoline and the similarity of its magnetic permeability. Capacitive approaches based on RC and RLC circuits demonstrate the ability to distinguish media with large permittivity contrasts, but are not yet able to consistently differentiate RON variations due to the narrow range of permittivity differences among gasoline types.

Overall, the results of this study confirm that methods for RON characterization must be aligned with the underlying chemical–structural parameters. 1H NMR spectroscopy possesses a more direct physical relevance to hydrocarbon molecular structure than simple sensor approaches based on electromagnetic responses. These findings provide a conceptual foundation for the development of more targeted fuel analysis methods and serve as a reference for evaluating the limitations of alternative approaches to RON characterization.

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