Predicting Sustainable Aviation Fuel Mixtures using Low-Resolution Nuclear Magnetic Resonance

Winford Janvrin* - Parker Huggins† - Austin R.J. Downey‡ - Sang Hee Won§

University of South Carolina, Columbia, SC 29208, USA

Sustainable aviation fuel (SAF) is a promising solution to mitigate the environmental impact of air travel. Because commercial jets contribute significantly to global greenhouse emissions, the accurate characterization of renewable and petroleum-based fuel mixtures is essential for ensuring regulatory compliance. Additionally, the implementation of in-situ fuel sensors allows for the continuous monitoring of fuel mixtures, enabling real-time quality control and enhanced engine performance. This paper explores the use of time-domain nuclear magnetic resonance (TD-NMR) to differentiate between mixtures of Jet A and Hydro-processed Renewable Jet (HRJ) Camelina. By analyzing ^{1}H TD-NMR relaxation data, we demonstrate a linear correlation between the decay rate and concentration of Jet A and HRJ Camelina mixtures. The fuel mixtures were tested using an open-source ^{1}H TD-NMR system developed by the authors that employs a 0.65 Tesla permanent magnet and operates at a Larmor frequency of 27.68 MHz. Results show that higher concentrations of Jet A yield slower relaxation rates. Furthermore, T_2 decay rate is shown to vary linearly with fuel composition, with correlation between the measured and synthesized relaxation rates of 11 mixtures of Jet A and HRJ Camelina achieving an R^2 value of 0.9845. The TD-NMR approach presented in this work provides a simple and efficient technique for on-site SAF characterization, an integral step towards facilitating the greater adoption of SAF and compliance with future regulations in the aviation industry.

I. Nomenclature

$TD\text{-}NMR$	=	Time Domain Nuclear Magnetic Resonance
NMR	=	Nuclear Magnetic Resonance
SAF	=	Sustainable Aviation Fuel
HRJ	=	Hydro-processed Renewable Jet
DCN	=	Derived Cetane Number
$CPMG$	=	Carr-Purcell-Meiboom-Gill
$RMSE$	=	Root Mean Squared Error
R^2	=	Coefficient of Determination
T_2	=	Transverse Relaxation Time
R_2	=	Transverse Relaxation Rate
PXI	=	PCI eXtensions for Instrumentation

---

*Undergraduate Research Assistant, Department of Mechanical Engineering

†Undergraduate Research Assistant, Department of Electrical Engineering

‡Associate Professor, AIAA Member, Department of Mechanical Engineering, Department of Civil, and Environmental Engineering, University of South Carolina, Columbia, SC 29208, USA, Contact Author austindowney@sc.edu

§Professor, Department of Mechanical Engineering

II. Introduction

The aviation industry is a significant contributor to global greenhouse gas emissions, accounting for 2.4% of the total in 2018 [1]. The demand for air travel is growing at a rapid rate, with the commercial jet fuel market predicted to grow from 71 billion gallons used to more than 230 billion globaly by 2050 [2]. As the market continues to grow, there is a rising effort to mitigate the environmental impact of aviation. By 2050, U.S. airlines are aiming to reduce carbon dioxide emissions by 50% compared to 2005 levels. Because low energy density batteries are a distant commercial option, sustainable aviation fuel (SAF) is a promising solution in the current time frame [3]. SAF has the potential to reduce greenhouse gas emissions by up to 80% compared to traditional jet fuels, thereby mitigating the aviation sector's impact on climate change [4]. To support the use of SAF, the Unites States Federal Government has launched the Sustainable Aviation Fuel Grand Challenge which aims to accelerate the production of SAF to meet 100% of commercial demand by 2050 [5].

Detecting the presence of SAF in general aviation fuel, or vice versa, is critical for several reasons, including regulatory compliance and operational efficiency. Accurate detection ensures that the environmental benefits of SAF are both realized and verifiable, further promoting SAF adoption. Additionally, regulatory bodies have stringent requirements and incentives for the use of SAF, making accurate detection essential for airlines to meet these standards and benefit from their associated financial incentives [6]. Given that SAFs vary in their chemical compositions and properties, precision fuel detection supports optimal engine function and promotes safety.

Nuclear magnetic resonance (NMR) is an analytical tool that exploits the magnetic properties of atomic nuclei. While high-resolution NMR spectroscopy is a powerful technique for analyzing the molecular structure of samples, time-domain NMR (TD-NMR) is a cost-efficient and versatile alternative [7]. Interest in using TD-NMR to directly probe the chemical properties of fuels has grown due to advancements in low-cost, low-field NMR systems [8]. For example, by analyzing T_2 relaxation times, Cunha et al. demonstrated that TD-NMR can detect adulteration of disel oil with kerosene, achieving excellent agreement with standard techniques such as mid-infrared spectroscopy [9]. Similarly, Rocha et al. developed a rapid and non-destructive TD-NMR-based method for determining biodiesel content in diesel–biodiesel blends, achieving high accuracing using both univariate and multivariate data analysis procedures [10]. Santos et al. explored TD-NMR as a rapid method for simultaneous assessment of quality parameters in commercial diesel samples, achieving accurate estimations of cetane index, density, and flash point [11].

The authors have also previously explored fuel characterization using TD-NMR. Martin et al. developed a prototype compact NMR system that utilizes a permanent magnet along with custom electronics and controls. Using the system, the initial strength of jet fuel T_2 curves was shown to correlate with hydrogen density, where measurements of hydrogen content achieved a maximum error of only 0.7% [12]. Huggins et al. proposed the use of TD-NMR in conjunction with interpretable machine learning to estimate the derived cetane number (DCN) of jet fuels directly from their T_2 relaxation curve. Using a random forest approach, results achieved a root mean squared error (RMSE) of just 0.96 DCN when predicting on new jet fuel samples [13].

In this work, the use of TD-NMR is explored to differentiate between mixtures of petroleum-derived and renewable jet fuels. By analyzing trends in the decay rate of T_2 relaxation curves, a linear correlation between the relaxation rate and composition of fuel mixtures is established. In this study, Jet A POSF 4658 and Hydro-processed Renewable Jet (HRJ) Camelina POSF 7720 are used for testing. Jet A, which is a kerosene-based fuel, is chosen for its widespread use in the U.S. aviation industry. HRJ Camelina, which is a SAF derived from Camelina plants [6], is chosen as a SAF test sample. The contribution of this work is twofold: (1) the demonstration that TD-NMR can effectively quantify the concentration of Jet A and HRJ Camelina mixtures, marking—to the knowledge of the authors—the first time TD-NMR has been explored for detecting SAF additives in petroleum-based fuel; and (2) the strong linear correlation ($R^2 = 0.9845$) established between measured and synthesized relaxation rates over a range of Jet A and HRJ Camelina mixtures.

III. Methodology

The open-source TD-NMR system used in this work is shown in Fig. 1 and was developed by the authors [14]. All of the custom electronics, barring a high-power amplifier, are housed on a single printed circuit board. The system is controlled by a LabVIEW program that interfaces with a National Instruments PXI system utilizing two arbitrary waveform generators (PXI-5421) and a data acquisition card (PXI-5122). The magnet design achieves a peak flux density of approximately 0.65 Tesla, yielding to a Larmor frequency of 27.68 MHz. Sample excitation is achieved using the Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence, and the T_2 relaxation curve of a sample is generated by plotting the peak of each spin echo against time.
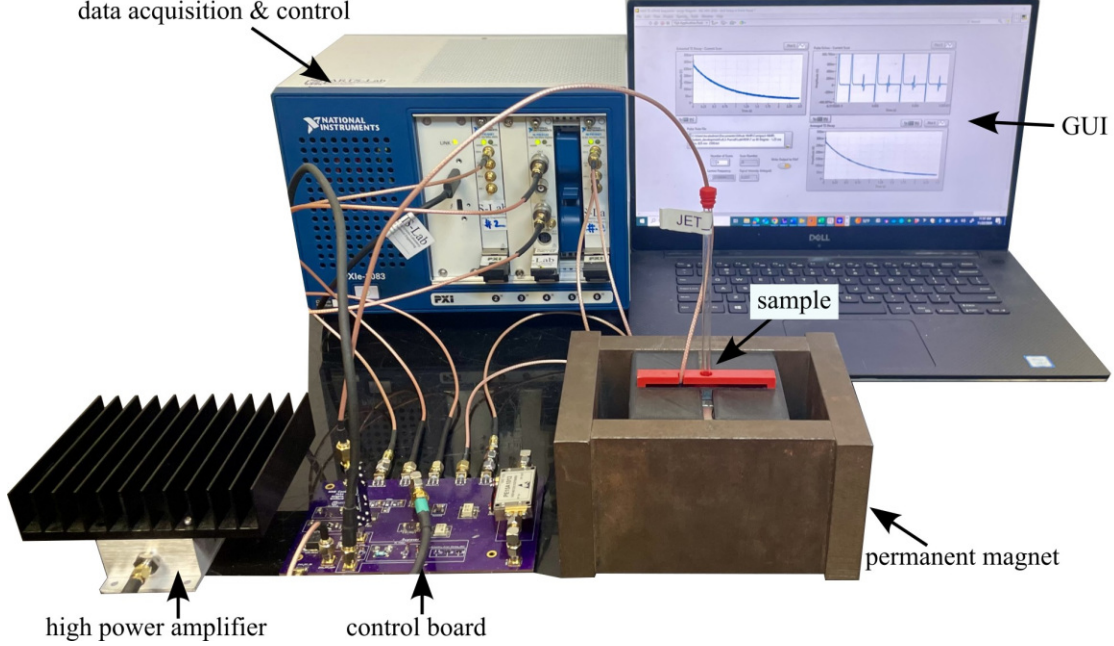
Fig. 1   Full compact TD-NMR system, with key components and subsystems annotated.

For experimentation, two sets of fuel mixtures were prepared in 10% mass increments, with each mixture having a total mass of 0.3 grams. For example, the samples included mixtures of 0.27 grams of Jet A with 0.03 grams of HRJ Camelina, 0.24 grams of Jet A with 0.06 grams of HRJ Camelina, and so forth. These mixtures, along with pure samples of Jet A and HRJ Camelina, were then probed using the introduced TD-NMR system. In total, the T_2 relaxation curves of 11 distinct mixtures were acquired five times, generating a dataset of 55 individual T_2 decay curves.

To each T_2 relaxation curve, we fit a first-order decaying exponential of the form

$$M_{\mathrm{xy}}(t) = M_0 \cdot \exp(-t/T_2), \tag{1}$$

where $M_{\mathrm{xy}}(t)$ is the magnetization at time t, M_0 is the initial magnetization, and T_2 is the spin-spin relaxation time. Note that the relaxation rate of a sample, R_2, is just the reciprocal of its relaxation time, i.e., $R_2 = 1/T_2$. To ensure the accuracy of measured relaxation rates, each T_2 relaxation curve was generated by averaging data from eight individual scans. Additionally, a low-pass moving median filter was applied to the acquired T_2 curves, removing high-frequency noise and further improving measurements of relaxation rate.

IV. Results

Fig. 2(a) shows the T_2 curves of mixtures prepared with increasing concentrations of Jet A. These results present the average of T_2 data acquired from five individual tests. It can be seen that the relaxation rates of the acquired decay curves decrease with increasing concentrations of Jet A. This observation is reflected in Fig. 2(b), where the relaxation rates of averaged T_2 curves are plotted against increasing concentrations of Jet A. For reference, the standard deviation of the measured relaxation rates are marked using black error bars.

To verify that changes in the relaxation rates of the mixtures can be predicted from the samples of Jet A and HRJ Camelina alone, synthetic relaxtion curves were generated by superimposing the decay curves of Jet A and HRJ Camelina as

$$M_{\mathrm{weighted}}(t) = C_{\mathrm{Jet}} \cdot M_{\mathrm{Jet}}(t) + C_{\mathrm{HRJ}} \cdot M_{\mathrm{HRJ}}(t), \tag{2}$$

where $M_{\mathrm{Jet}}(t)$ is the relaxation curve of Jet A, $M_{\mathrm{HRJ}}(t)$ is the relaxation curve of HRJ Camelina, and $0 \le C_{\mathrm{Jet}}, C_{\mathrm{HRJ}} \le 1$ are the concentrations of Jet A and HRJ Camelina, respectively. Fig. 3(a) reports the 11 experimental fuel samples as blue markers, with each sample's measured R_2 value on the horizontal axis and the corresponding synthesized R_2 value (obtained from Equation 2) on the vertical axis. A clear linear relationship between the measured and synthesized relaxation rates is present, with the line of best fit achieving an R^2 value of 0.9845. Fig. 3(b) shows the fitting error
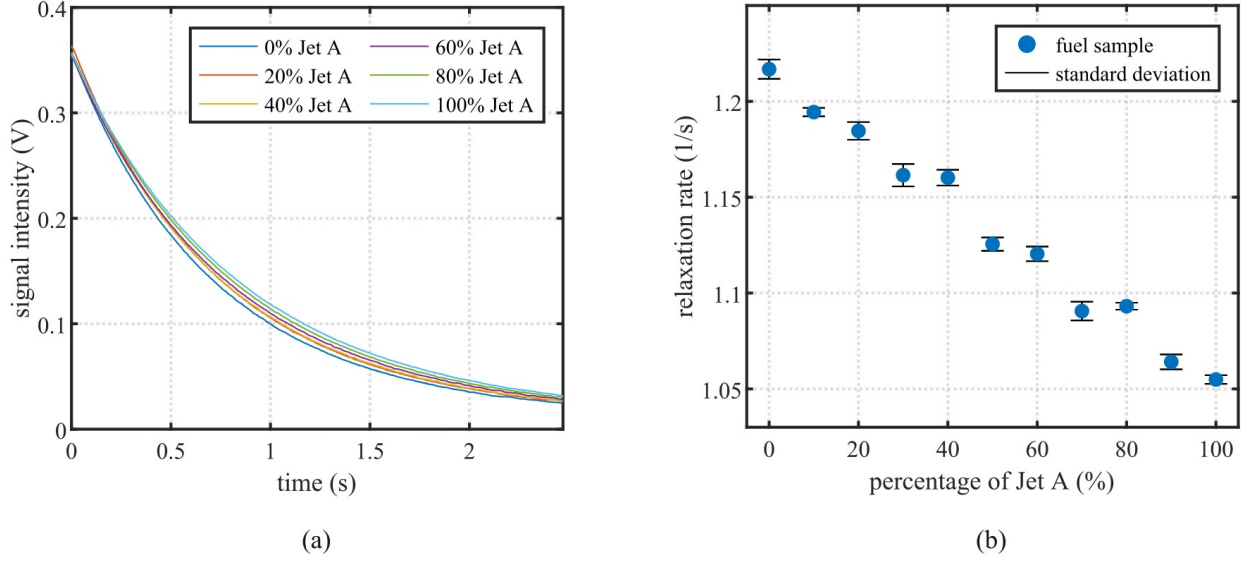
Fig. 2   Relaxation data for mixtures of Jet A and HRJ Camelina. (a) Averaged T_2 curves from five individual acquisitions. (b) Averaged relaxation rates against concentrations of Jet A.
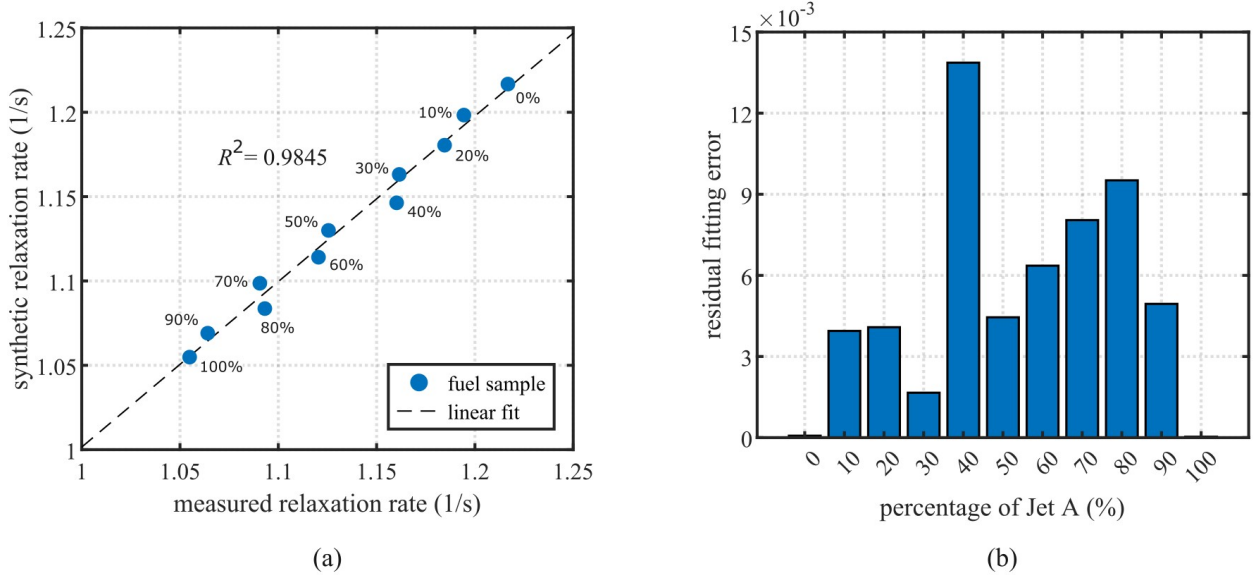
Fig. 3   Relaxation rates for both measured and synthetic fuel mixtures. (a) Linear correlation between measured and synthetic decay rates. (b) Residual fitting error for different concentrations of Jet A.

between each tested mixture and the proposed linear model. The observed errors can be primarily attributed to human error during sample preparation, specifically to the challenges associated with accurately mixing small volumes of fuel. Additionally, minor variations in the NMR system, including temperature-induced changes affecting the magnetic field strength and slight calibration discrepancies, contribute to the overall measurement imprecision.

V. Conclusion

This study demonstrates the effectiveness of TD-NMR in detecting and quantifying SAF within jet fuel blends. By examining the T_2 relaxation curves of various fuel samples, a strong linear correlation was established between the relaxation rate and composition of Jet A and HRJ Camelina mixtures. This high degree of linearity, evidenced

by a R^2 value of 0.9845, indicates that low-resolution TD-NMR is a promising method for distinguishing between conventional and renewable jet fuels. Given that the ability to accurately quantify SAF concentrations is essential for meeting regulatory requirements and optimizing engine performance, the proposed TD-NMR approach offers a practical solution for on-site fuel characterization. Future work will focus on the implementation of flow-through NMR, enabling the SAF detection process to be streamlined and integrated into fuel distribution networks. Additionally, a broader range of SAF-based mixtures will be explored, and the sources of error identified in this work will be addressed. The resulting advancements in fuel detection technology will support the broader goal of reducing the aviation industry's environmental impact by promoting the adoption of sustainable fuels.

Acknowledgments

References

[1] Graver, B., Zhang, K., and Rutherford, D., "Emissions from commercial aviation, 2018," *International Council on Clean Transportation*, 2019.

[2] U.S. Energy Information Administration EIA, "Annual Energy Outlook 2023 Table 47," , 2023.

[3] Holladay, J., Abdullah, Z., and Heyne, J., *Sustainable Aviation Fuel: Review of Technical Pathways*, 2020. https://doi.org/10.2172/1660415.

[4] Overton, J., "An Introduction to Sustainable Aviation Fuels: Part 1 of a series,'Sustainable Aviation Fuels: A Critical Emissions Mitigation Strategy Gaining Momentum'," *online:< https://www. eesi. org/articles/view/an-introduction-to-sustainableaviation-fuels*, 2022.

[5] House, W., "FACT SHEET: Biden administration advances the future of sustainable fuels in American aviation," https://www.whitehouse.gov/briefing-room/statements-releases/2021/09/09/fact-sheet-biden-administration-advances-the-future-of-sustainable-fuels-in-american-aviation/, 2021.

[6] Shila, J., and Johnson, M. E., "Techno-economic analysis of Camelina-derived hydroprocessed renewable jet fuel within the US context," *Applied Energy*, Vol. 287, 2021, p. 116525. https://doi.org/10.1016/j.apenergy.2021.116525.

[7] Kruk, D., and Florek-Wojciechowska, M., *Recent development in 1H NMR relaxometry*, Elsevier, 2020, pp. 119–184. https://doi.org/10.1016/bs.arnmr.2019.10.001.

[8] Nikolskaya, E., and Hiltunen, Y., "Time-Domain NMR in Characterization of Liquid Fuels: A Mini-Review," *Energy and Fuels*, Vol. 34, No. 7, 2020, pp. 7929–7934. https://doi.org/10.1021/acs.energyfuels.0c01464.

[9] Cunha, D. A., Montes, L. F., Castro, E. V., and Barbosa, L. L., "NMR in the time domain: A new methodology to detect adulteration of diesel oil with kerosene," *Fuel*, Vol. 166, 2016, pp. 79–85. https://doi.org/10.1016/j.fuel.2015.10.078.

[10] da Rocha, G., Colnago, L. A., Moraes, T. B., Zagonel, G. F., de Muniz, G. I. B., Peralta-Zamora, P. G., and Barison, A., "Determination of Biodiesel Content in Diesel Fuel by Time-Domain Nuclear Magnetic Resonance (TD-NMR) Spectroscopy," *Energy and Fuels*, Vol. 31, No. 5, 2017, pp. 5120–5125. https://doi.org/10.1021/acs.energyfuels.6b03508.

[11] Santos, P. M., Amais, R. S., Colnago, L. A., Rinnan, A., and Monteiro, M. R., "Time Domain-NMR Combined with Chemometrics Analysis: An Alternative Tool for Monitoring Diesel Fuel Quality," *Energy and Fuels*, Vol. 29, No. 4, 2015, pp. 2299–2303. https://doi.org/10.1021/acs.energyfuels.5b00017.

[12] Martin, J., Downey, A., and Won, S. H., "Compact Time Domain NMR Design for the Determination of Hydrogen Content in Gas Turbine Fuels," *Volume 1: 24th International Conference on Advanced Vehicle Technologies (AVT)*, American Society of Mechanical Engineers, 2022. https://doi.org/10.1115/detc2022-90023.

[13] Huggins, P., Martin, J., Downey, A. R., and Won, S. H., "Interpretable Machine Learning for Predicting Derived Cetane Number of Jet Fuels Using Compact TD-NMR," *Available at SSRN 4928292*, 2024.

[14] ARTS-Lab, "Compact-NMR," GitHub, 2024. URL https://github.com/ARTS-Laboratory/Compact-NMR.