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

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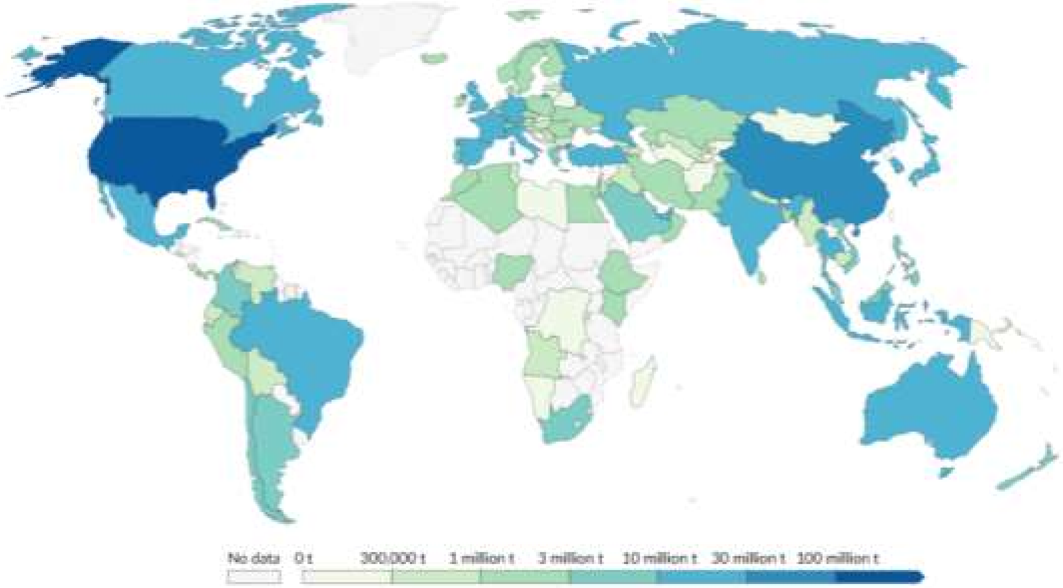
Aviation’s Environmental Impact

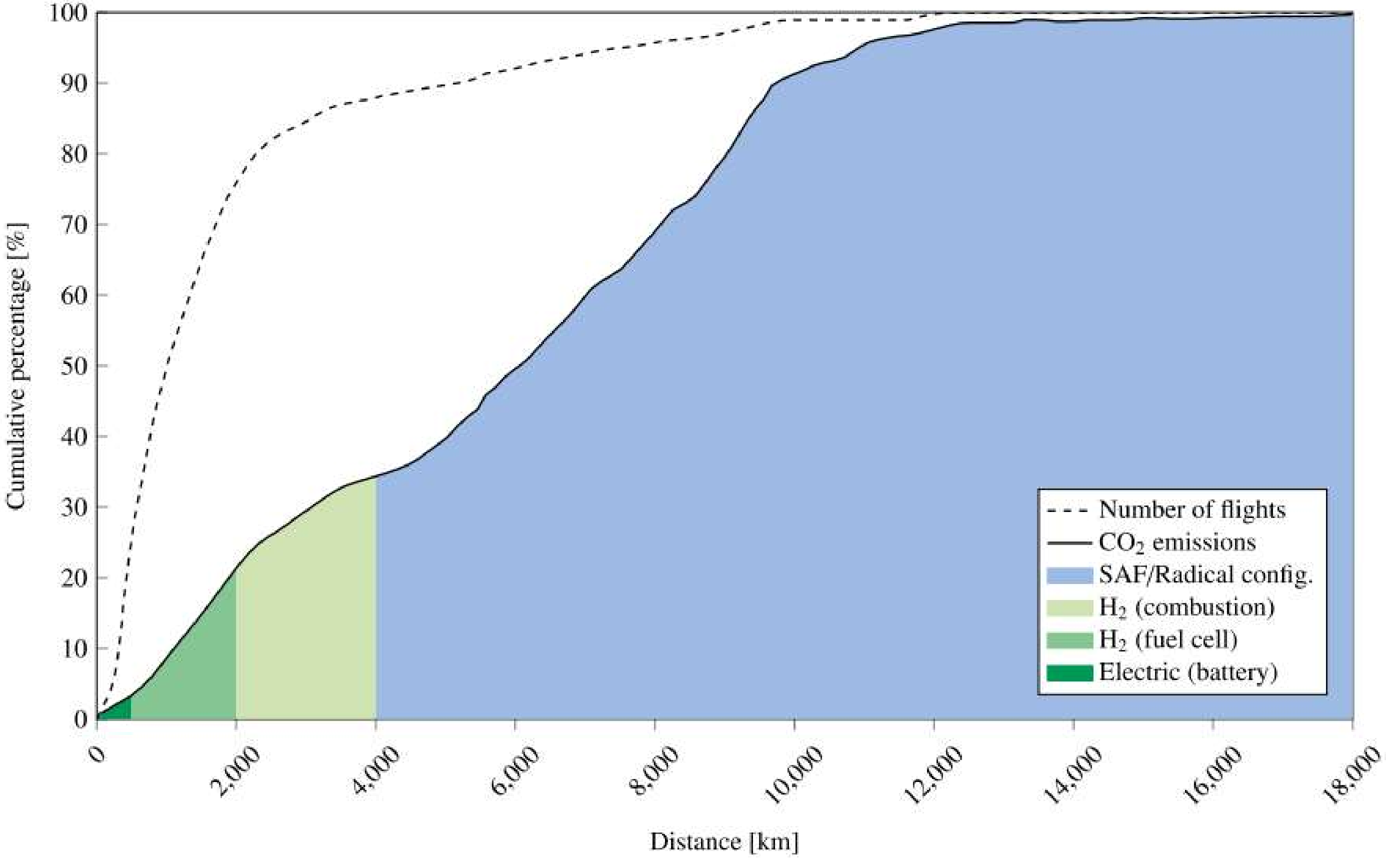
- The Aviation industry accounted for 2.4% of total green house gas emissions in 2018.
- The demand for jet fuel is projected to grow from 71 billion gallons to over 230 billion gallons by 2050, emphasizing the need for sustainable solutions.
- Sustainable Aviation Fuel (SAF) offers a transformative opportunity, reducing greenhouse gas emissions by up to 80% compared to traditional jet fuels.



OurWorldinData.org/co2-and-greenhouse-gas-emissions | CC BY

Sustainable Aviation Fuel (SAF)

- Sustainable aviation fuel (SAF) is a biofuel that can be used in place of conventional jet fuel to power aircraft
- SAF offers a transformative opportunity, reducing greenhouse gas emissions by up to 80% compared to traditional jet fuels.



Svensson, Christian, Amir AM Oliveira, and Tomas Grönstedt. "Hydrogen fuel cell aircraft for the Nordic market." *International Journal of Hydrogen Energy* 61 (2024): 650-663.

The Case for SAF Detection

- The United States has launched the Sustainable Aviation Fuel Grand Challenge aiming to accelerate the production of SAF to meet 100% of commercial demand by 2050.
- Accurate detection of SAF ensures:
  - Compliance with stringent regulations.
  - Achievement of intended environmental benefits.
  - Optimization of engine performance.
  - Supporting widespread adoption in the aviation industry.

Rolls-Royce engine compatible with 100% Sustainable Aviation Fuel

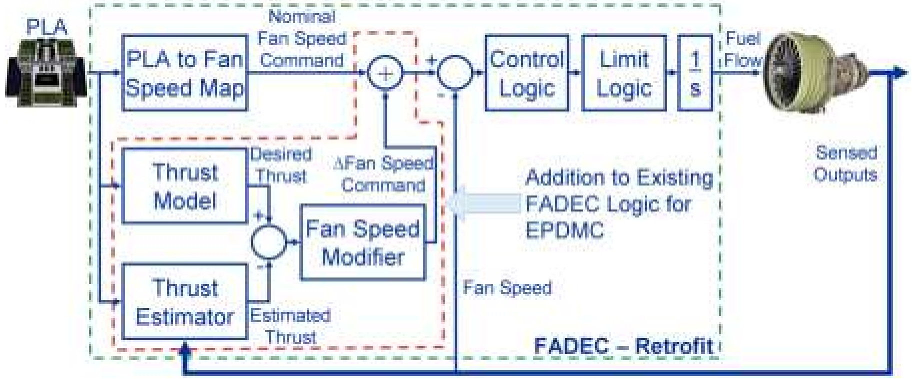
Credit: Rolls-Royce

Team Goals (now and future)

1. Rapidly differentiate between mixtures of petroleum-derived and renewable jet fuels.
2. Create a cost-effective on-site fuel monitoring system.
3. Develop sensors for advanced engine control, potentially for dynamic mixtures of SAF and kerosene.

Approach:

- Time domain nuclear magnetic resonance relaxometry (TD-NMR) using a CPMG sequence
- Inexpensive compared to High-field NMR spectroscopy and portable.

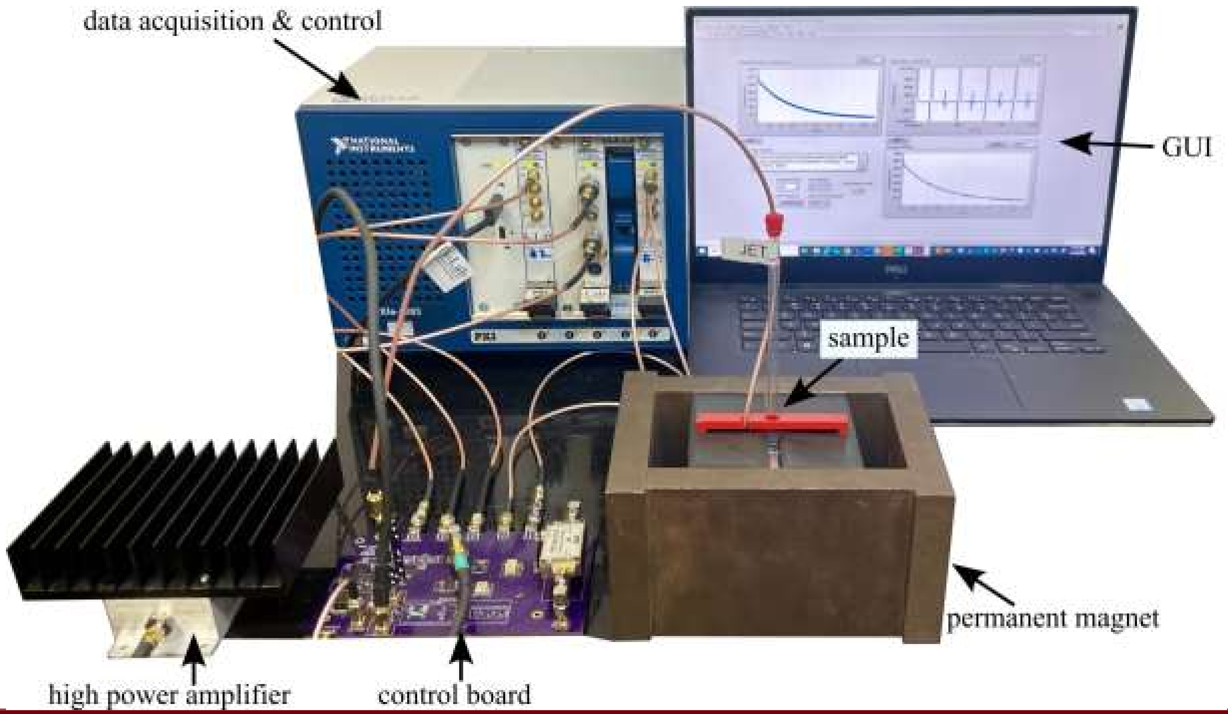


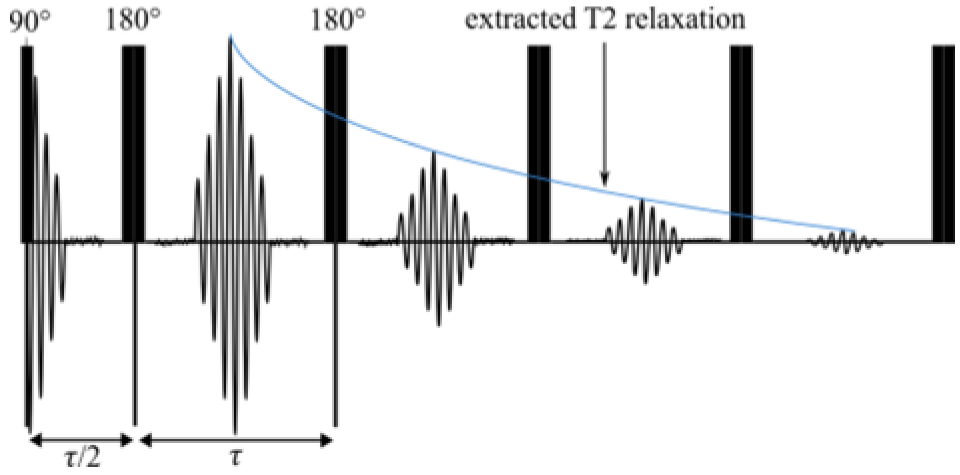
Typical Current Engine Control

Fundamentals of Aircraft Turbine Engine Control, Dr. Sanjay Garg Chief, Controls and Dynamics Branch, NASA

ARTS-Lab desktop NMR system

- Control handled by LabVIEW program and NI-PXI chassis
- All electronics (barring one amplifiers) housed on a single PCB
- GUI developed for easy data acquisition and export

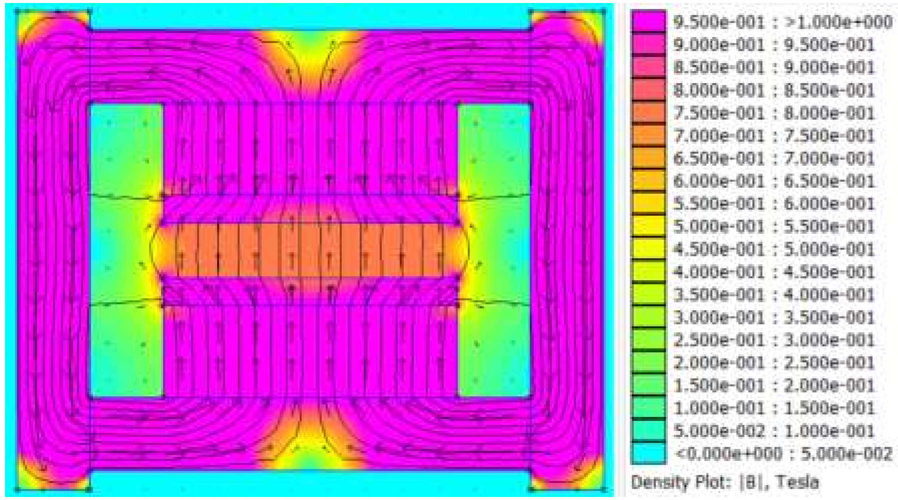




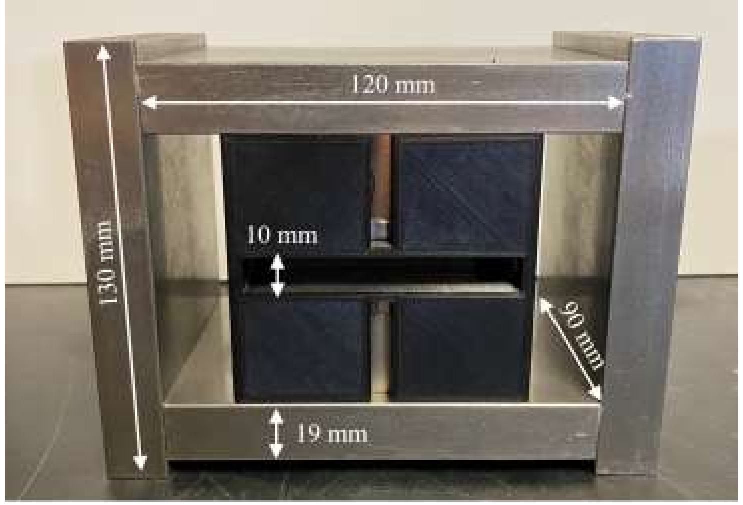
Extraction of T2 relaxation curve using a CPMG sequence

Permanent magnet array

- N42 cylindrical dipole magnets enclosed by a steel yolk
- 1018 carbon steel caps affixed to magnet surfaces
- Peak flux density of 0.645 T → Larmor frequency of 27.5 MHz
- Temperature shift gradient of -800 ppm/K



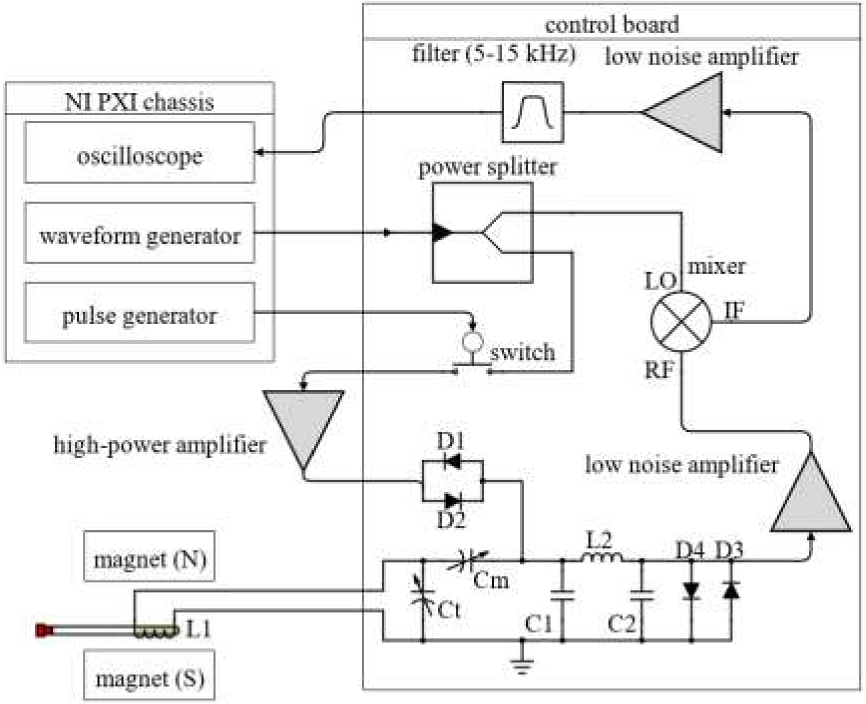
Simulation of magnet flux density



Magnet dimensions

RF electronics

- A single 24 V DC power supply required
- Impedance of all cables and PCB traces matched to 50 Ω
- Waveform generator → sine wave at Larmor frequency
- Pulse generator → CPMG pulse train
- Duplexer (crossed diodes) isolates probe and LNA

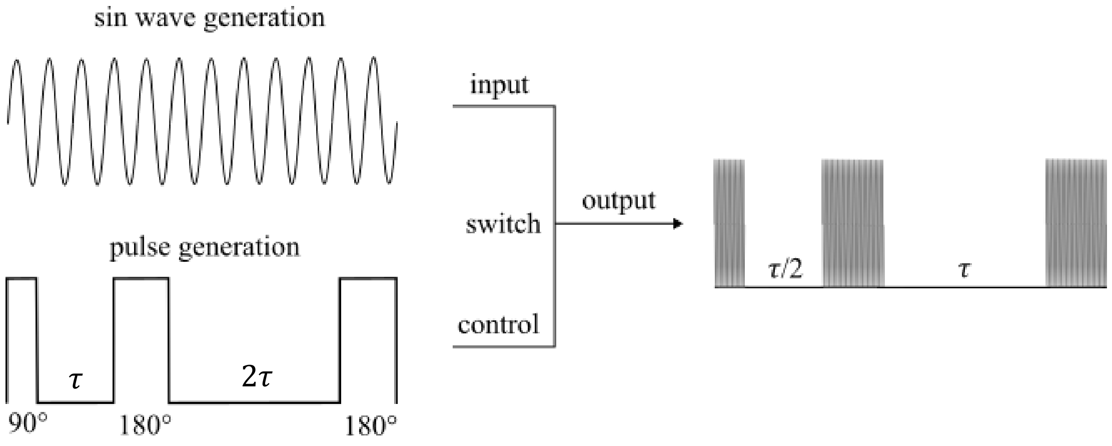


General flow

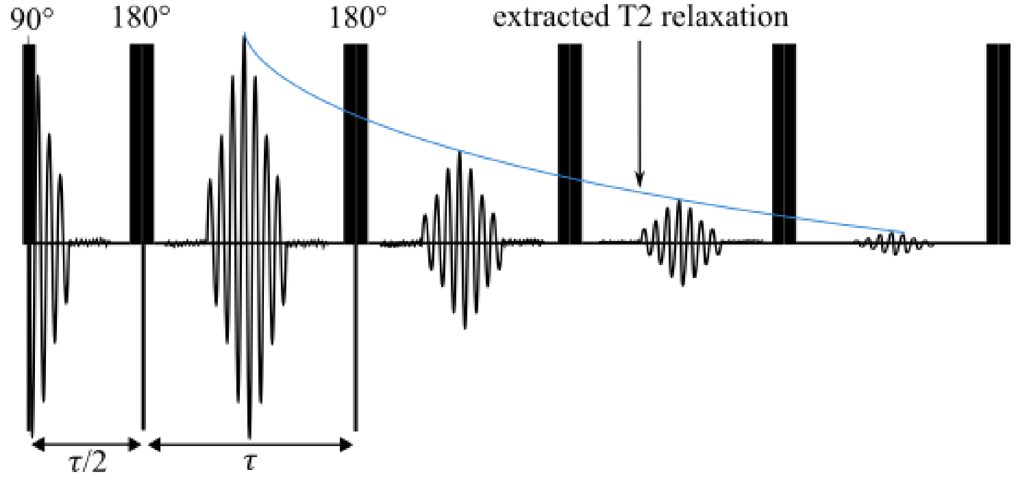
excitation → NMR response → amplification → mixing → filtering

Signal generation and control

- NI PXI chassis
  - Arbitrary waveform generator
  - Pulse train generator
  - 16-bit digitizer



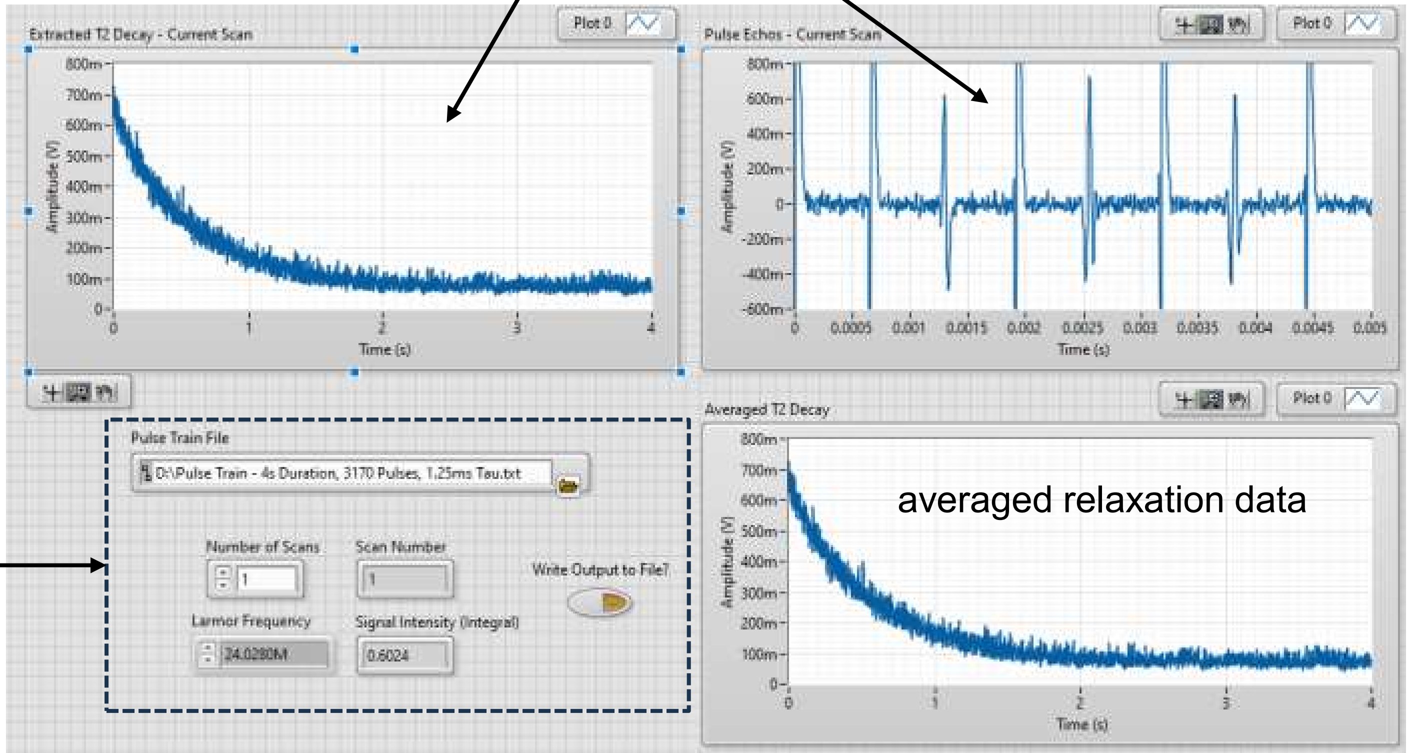
- CPMG pulse train
  - 3955 total pulses
  - 90° pulse duration is 7 μs
  - $\tau = 0.625$ ms



Data acquisition

- LabVIEW GUI serves as front end
- Each test comprises 8 scans (average)
- Time for T_2 curve acquisition < 1 min
- Thermocouple used for frequency calibration

current scan outputs



Pulse Train File: D:\Pulse Train - 4s Duration, 3170 Pulses, 1.25ms Tau.txt

Number of Scans: 1

Scan Number: 1

Larmor Frequency: 24.0280M

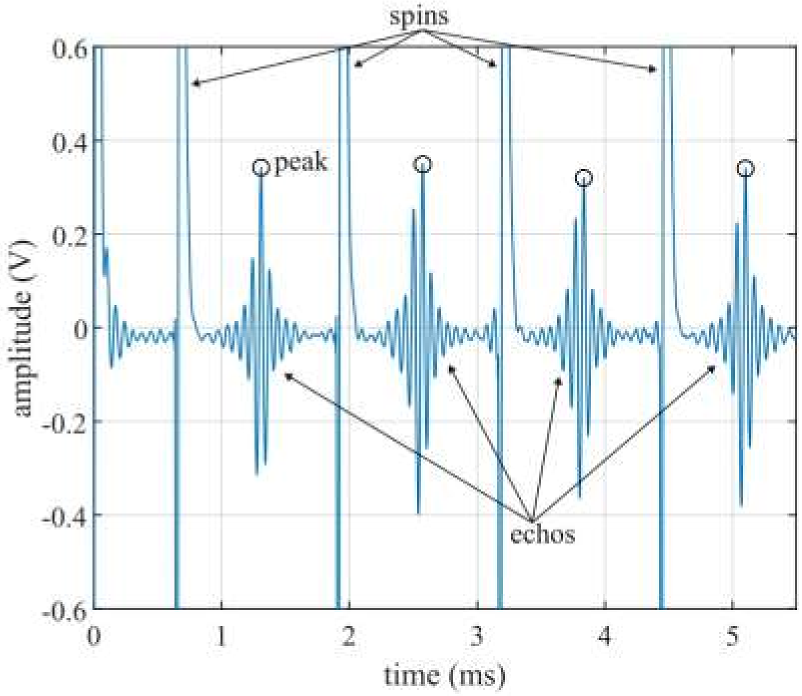
Signal Intensity (Integral): 0.6024

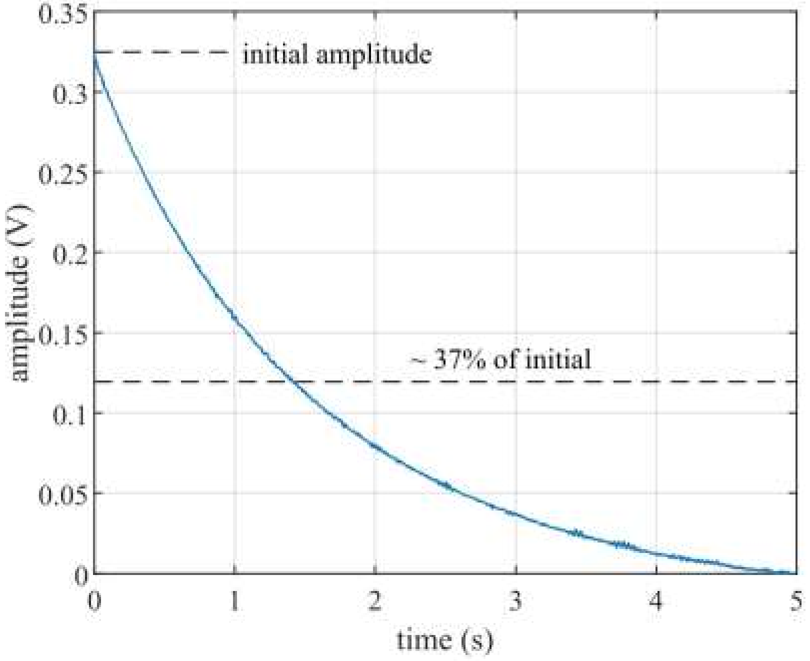
user adjustable parameters

averaged relaxation data

TD-NMR signal and T_2

- T_2 relaxation modeled as $M_{\mathrm{xy}}(t) = M_0 \exp(-t/T_2)$
- Relaxation rate is the reciprocal of relaxation time (i.e., $R_2 = 1/T_2$)
- Linear relationship between R_2 and hydrogen content well established



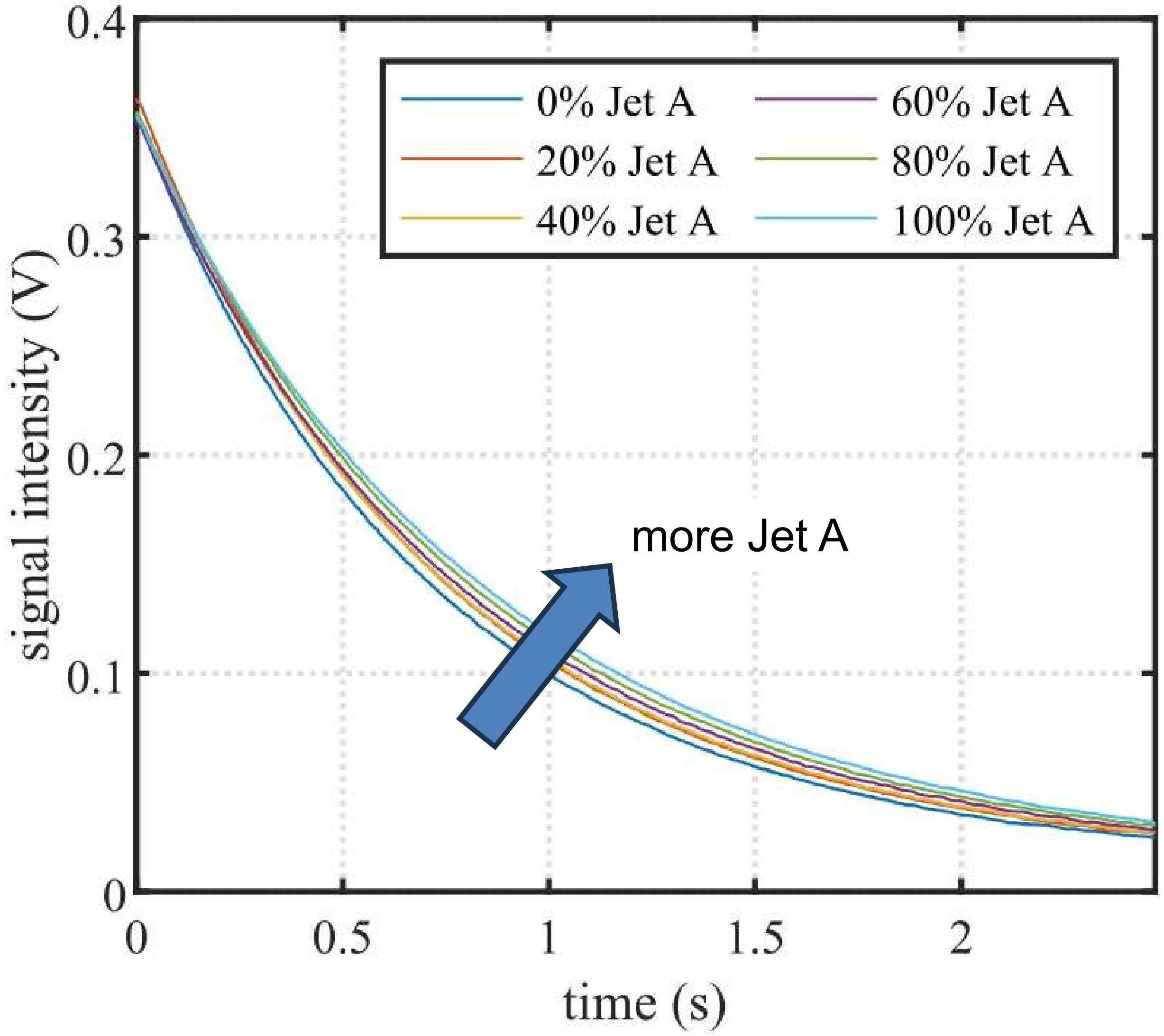


Sample preparation

- Fuel mixture sets of Jet A and HRJ Camelina were created in 10% mass increments, with each mixture totaling 0.3 grams.
    - Ex. 0.27 grams Jet A, 0.03 grams HRJ Camelina
- 11 distinct mixtures including pure samples of Jet A and HRJ Camelina were probed five times, generating a dataset of 55 T_2 curves.

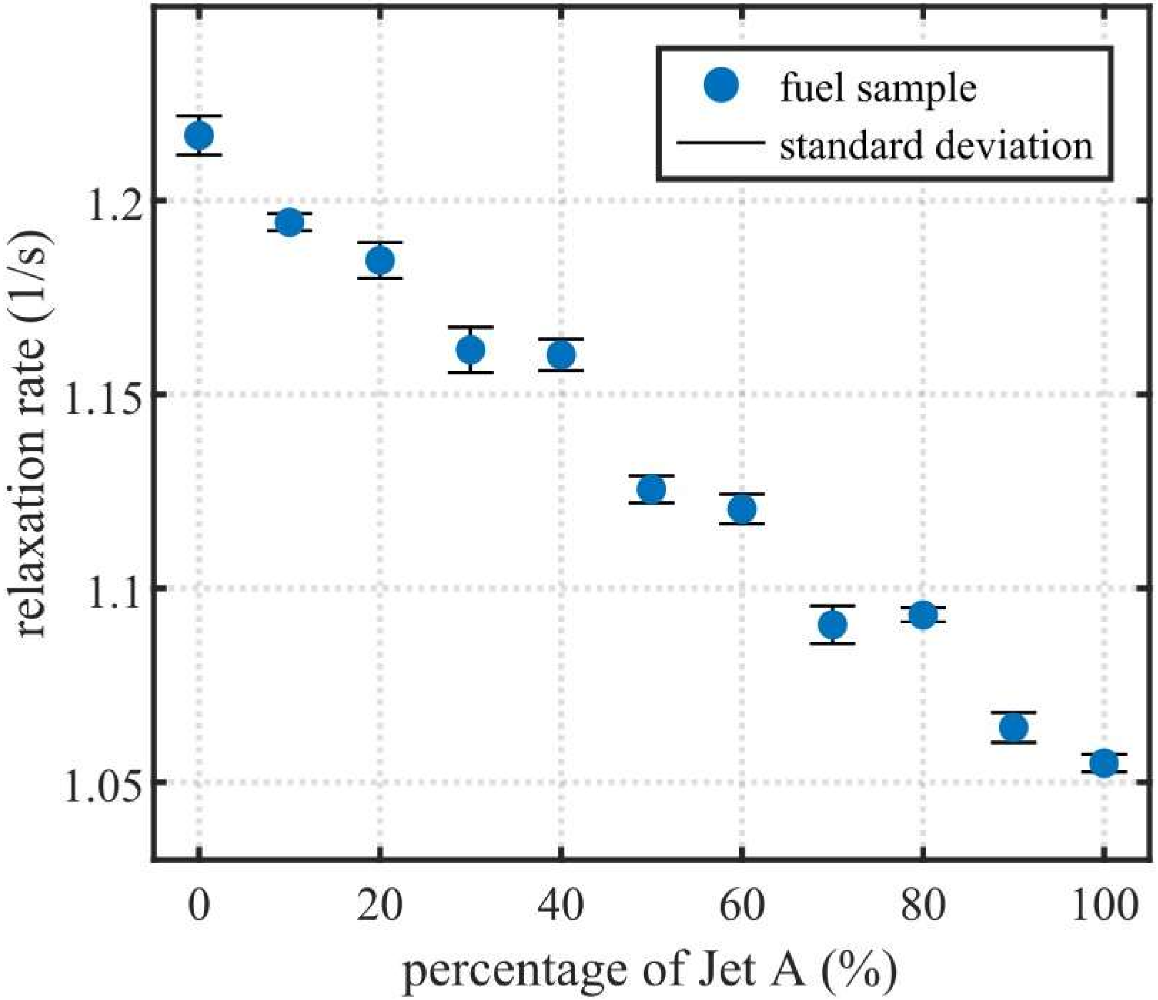
Relaxation rate analysis

- The averaged T_2 data is shown in figure (a) for 6 different concentrations of Jet A and HRJ Camelina.
- It was observed that the relaxation rates decrease with increasing concentrations of Jet A.



SAF Relaxation rate vs concentration

- Relaxation rates decrease with increasing Jet A concentration, reflecting a link between composition and TD-NMR response.
- A strong linear correlation ($R^2 = 0.9845$) between measured and synthetic relaxation rates confirms TD-NMR's reliability for quantifying SAF concentrations.



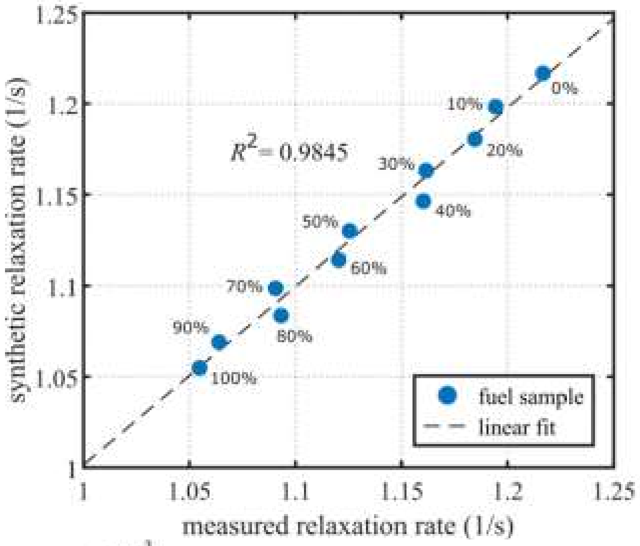
Predicting mixtures

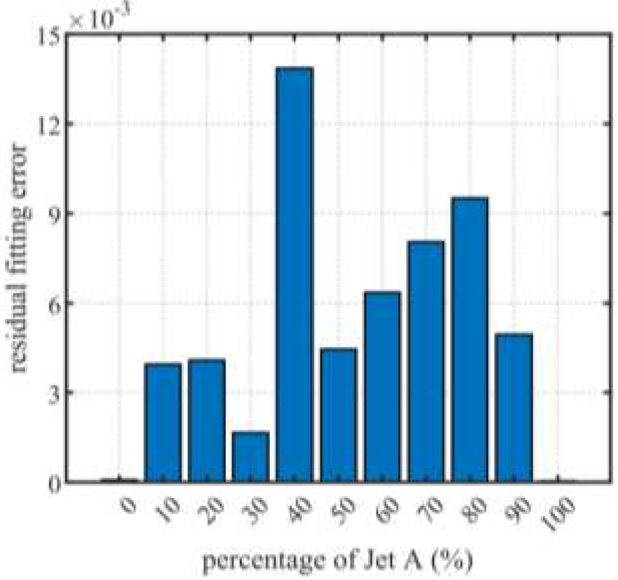
- Synthetic relaxation curves were generated by superimposing the decay curves of Jet A and HRJ Camelina as:

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

where $M_{\text{Jet}}(t)$ is the relaxation curve of Jet A, $M_{\text{HRJ}}(t)$ is the relaxation curve of HRJ Camelina, and $0 \leq C_{\text{Jet}}, C_{\text{HRJ}} \leq 1$ are the concentrations of Jet A and HRJ Camelina, respectively.

- The top figure shows each sample's measured R_2 value on the horizontal axis and the corresponding synthesized value on the vertical axis. A linear relationship was found achieving an R^2 of 0.9845.
- Fitting error is shown in the bottom figure and is attributed to human error during preparation and mixing small volumes of fuel.





Conclusion

- Time-domain nuclear magnetic resonance (TD-NMR) is a cost-effective and reliable tool for analyzing Sustainable Aviation Fuel (SAF) mixtures.
- The system developed is compact, open-source, and adaptable, enabling widespread use across industries.
- High accuracy and linear correlation demonstrate the potential for real-time, on-site SAF monitoring.
- Future work includes integrating flow-through systems for continuous monitoring and exploring broader applications like material science and food safety.

Credit: Envato Elements CC

THANKS!

National Science Foundation

Compact-NMR (cNMR)

Our design is open source and available on GitHub!

https://github.com/ARTS-Laboratory/Compact-NMR

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