Water Quality Monitoring using Field Deployable NMR

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UNIVERSITY OF
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The ARTS-Lab at USC

We use

foundational science

Day School

to develop essential tools

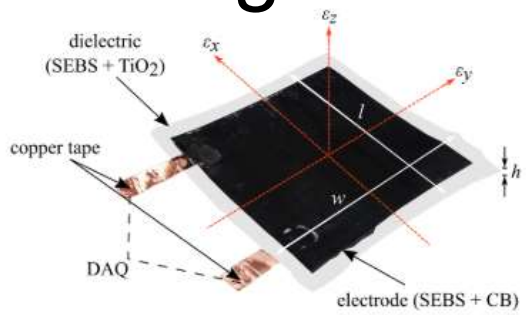
Dan Thompson

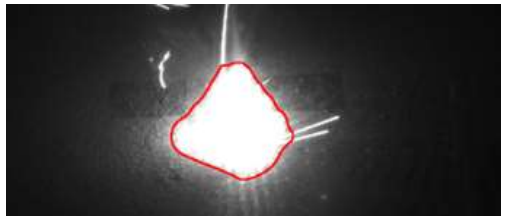
to solve real-world problems

public domain

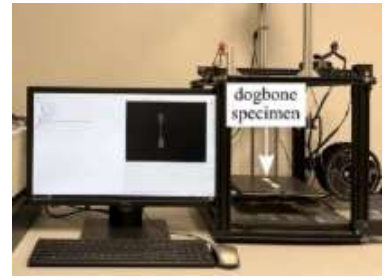
We are Engineers (mostly)

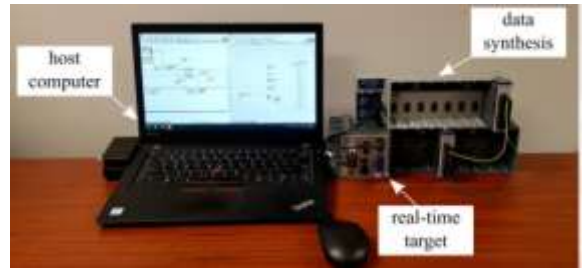
Sensing

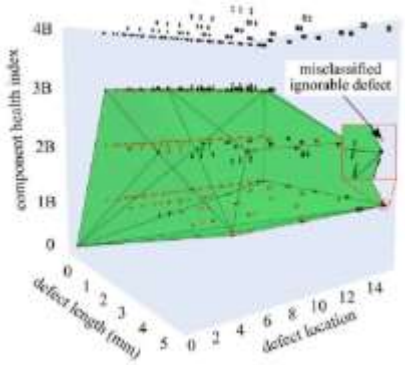


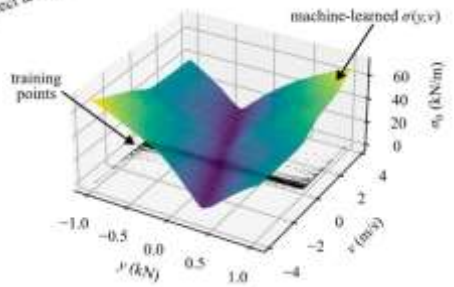


Data Assimilation

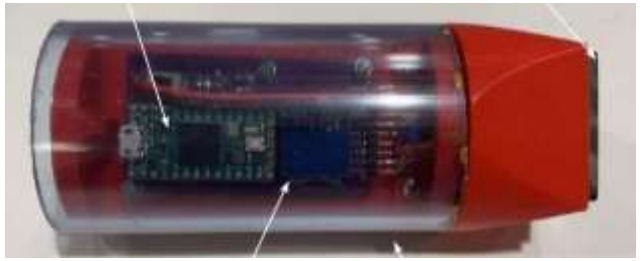








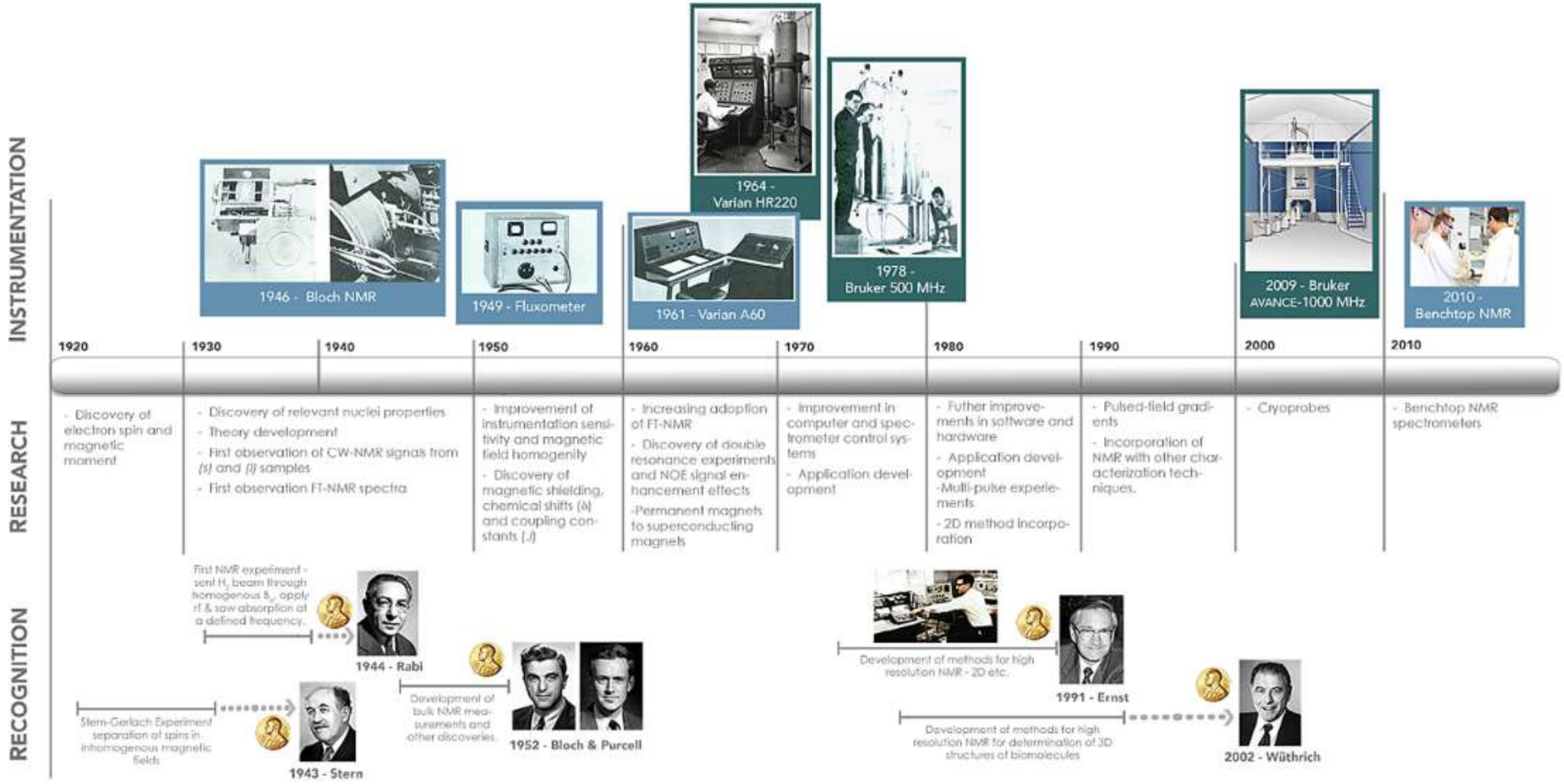
AI/ML



Embedded Systems

Water Quality Monitoring using Field Deployable NMR

History of NMR

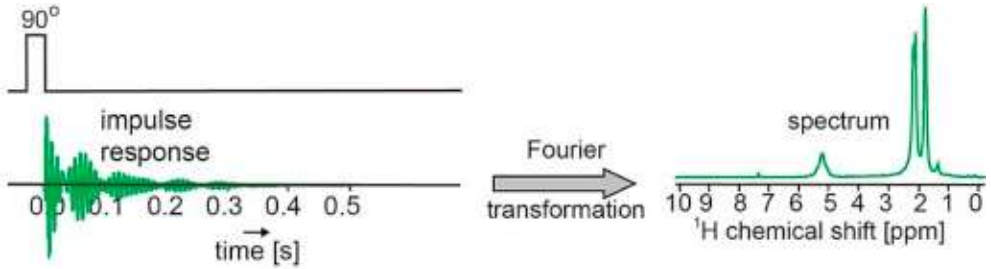


Riegel, Susanne D., and Garett M. Leskowitz. "Benchtop NMR spectrometers in academic teaching." TrAC Trends in Analytical Chemistry 83 (2016): 27-38.

Nuclear Magnetic Resonance (NMR) Techniques

NMR spectroscopy

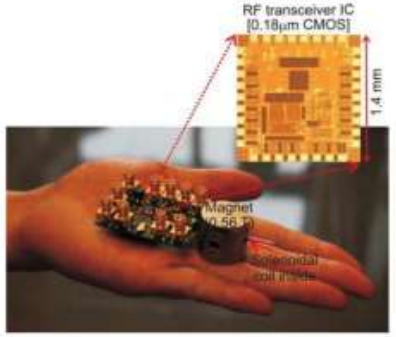
- Lab-Grade NMR
  - Frequency domain analysis
  - High resolution
  - Expensive & bulky

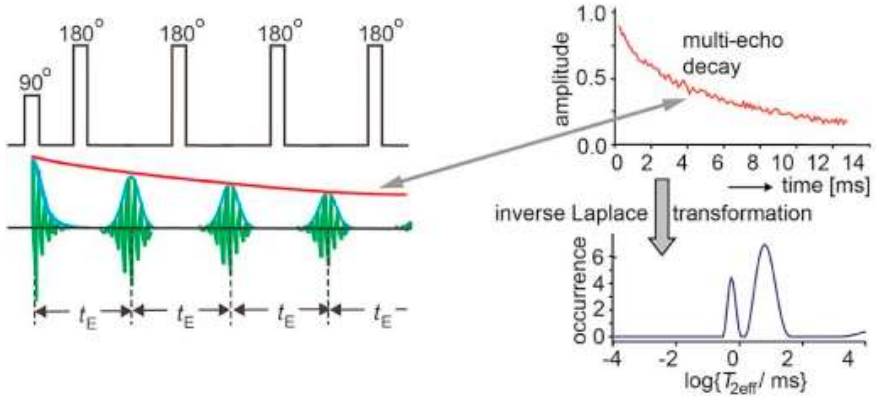


B. Blümich, “Introduction to compact NMR: A review of methods,” TrAC Trends in Analytical Chemistry, vol. 83, pp. 2–11, Oct. 2016.

NMR Relaxometry

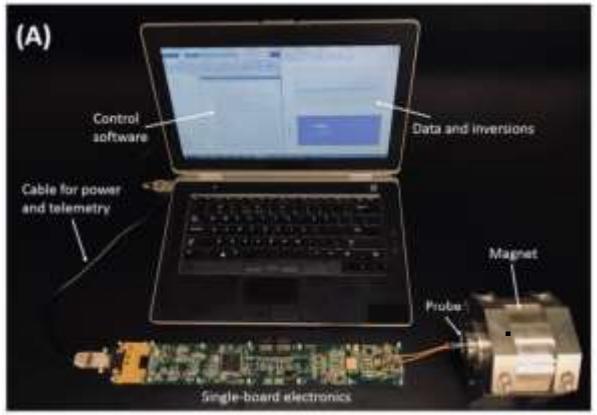
- Low-field NMR relaxometry
  - Time domain analysis
  - Low resolution
  - Inexpensive and portable



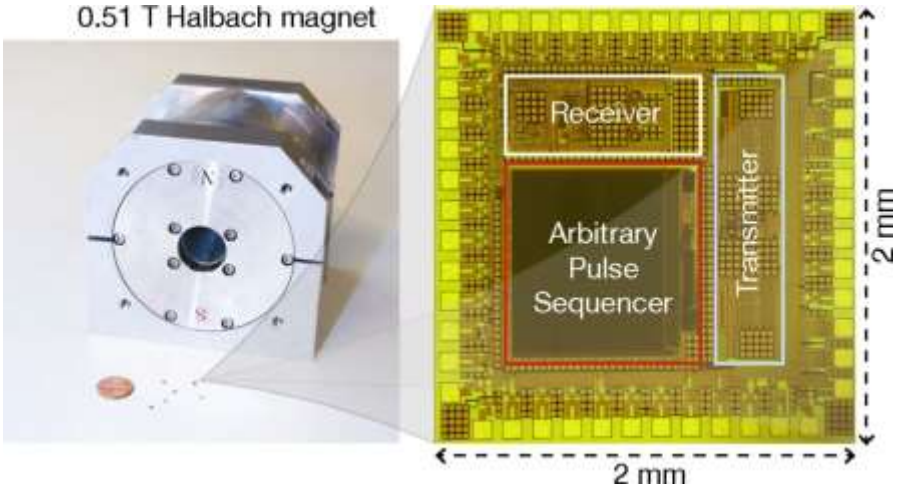


B. Blümich, “Introduction to compact NMR: A review of methods,” TrAC Trends in Analytical Chemistry, vol. 83, pp. 2–11, Oct. 2016.

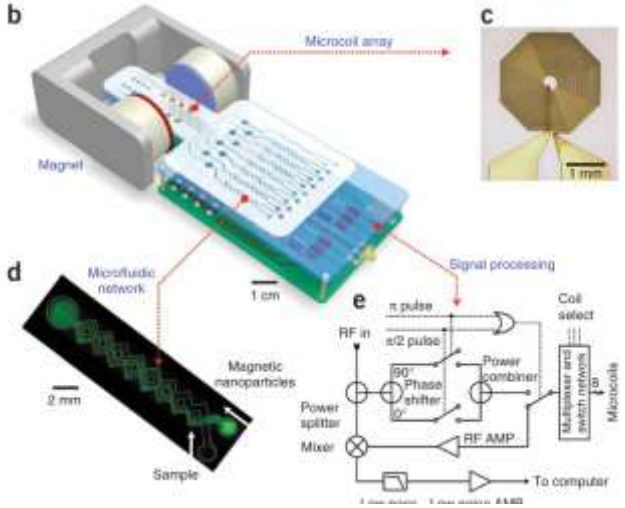
Miniature NMR systems



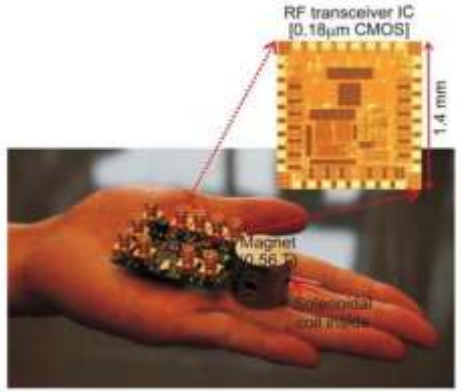
Tang, Yiqiao, David McCowan, and Yi-Qiao Song. "A miniaturized spectrometer for NMR relaxometry under extreme conditions." Scientific reports 9.1 (2019): 11174



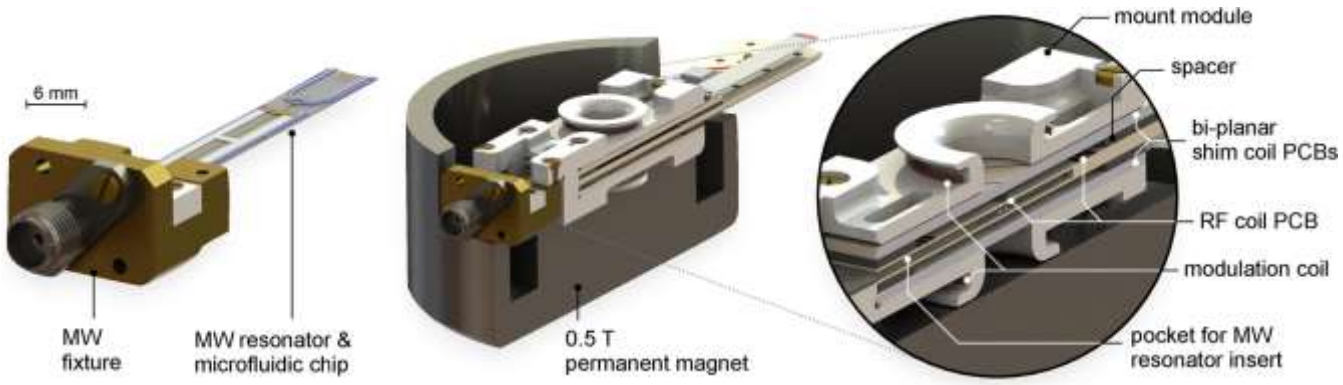
https://physicsworld.com/a/going-mobile-with-nmr-spectroscopy/



Lee, Hakho, et al. "Chip–NMR biosensor for detection and molecular analysis of cells." *Nature medicine* 14.8 (2008): 869-874.



Sun, Nan, et al. "Palm NMR and 1-chip NMR." *IEEE Journal of Solid-State Circuits* 46.1 (2010): 342-352.

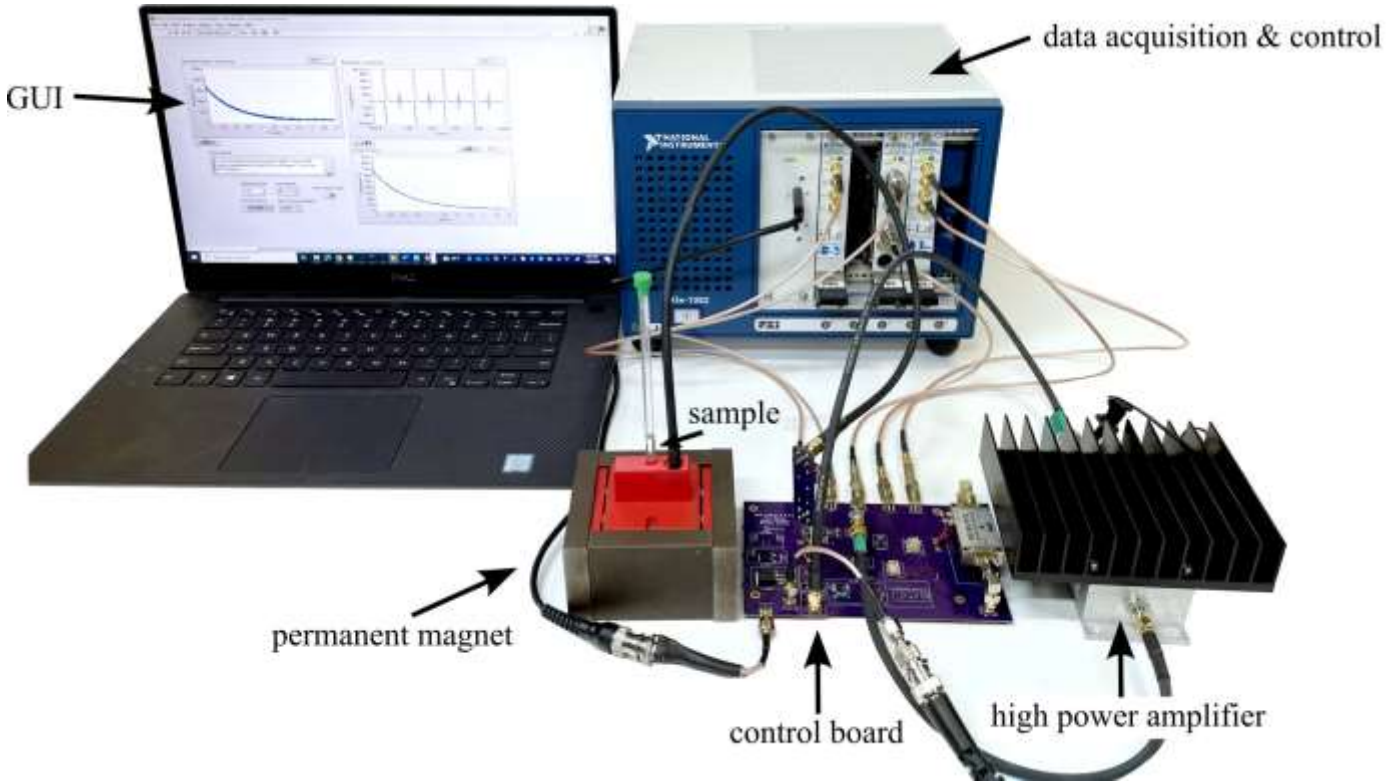


Lee, Hakho, et al. "Chip–NMR biosensor for detection and molecular analysis of cells." *Nature medicine* 14.8 (2008): 869-874.

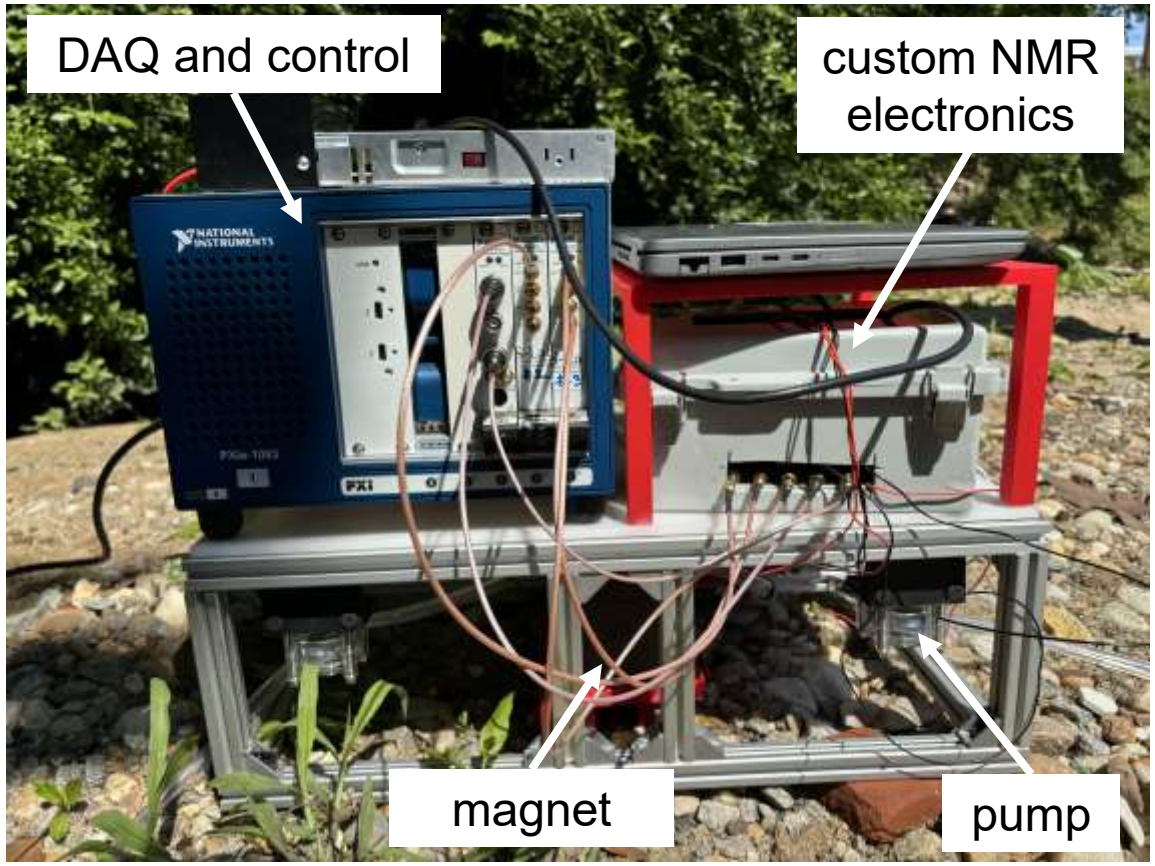
Our Open-source NMR System

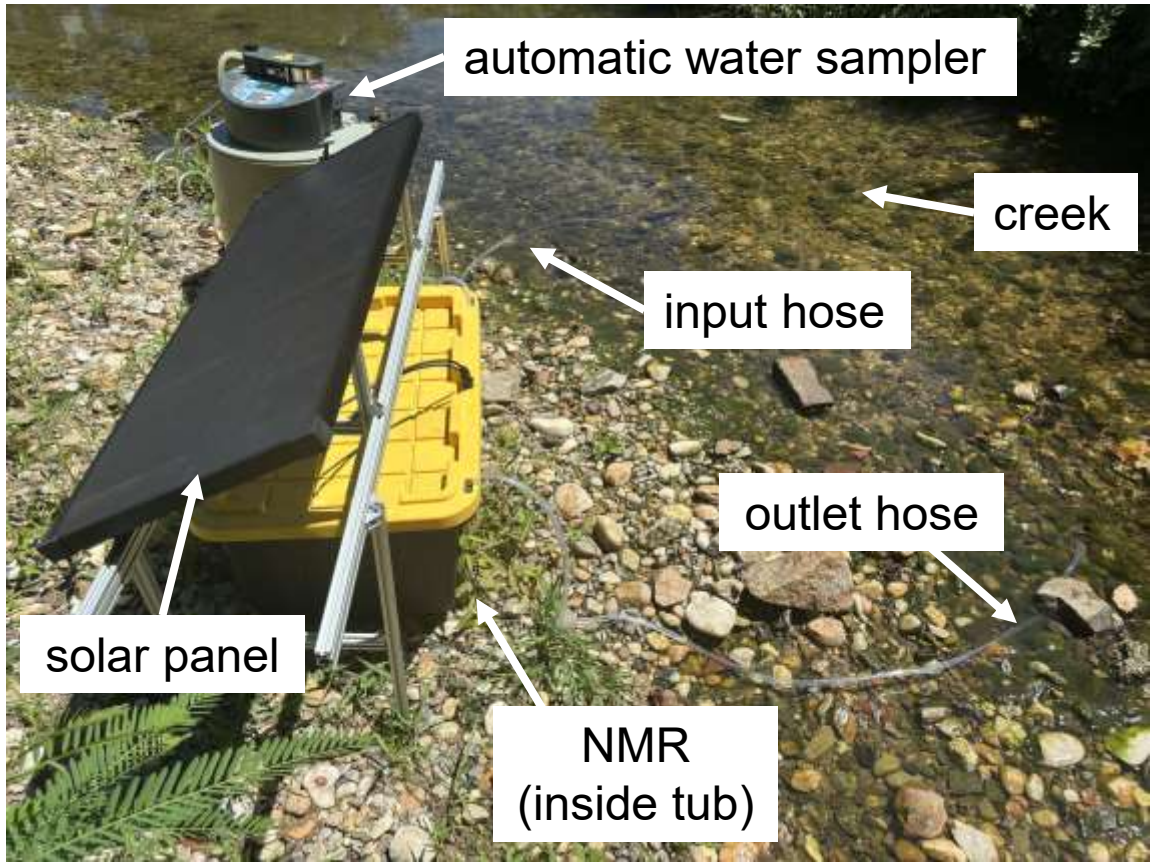
ARTS-Lab Desktop NMR System

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



Flow-through NMR





Past NMR Development

2019 2020 2021 2022 2023 2024 2025

Funding

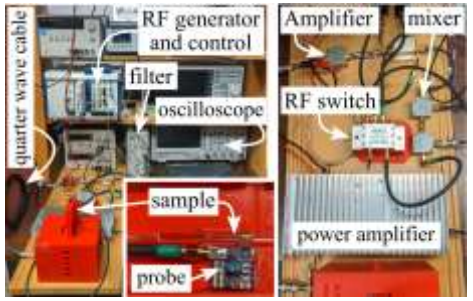
Downey/San Hee | Army | USC | NSF CA

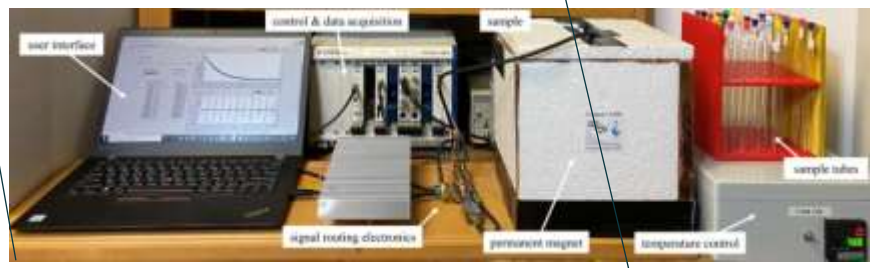
Hardware

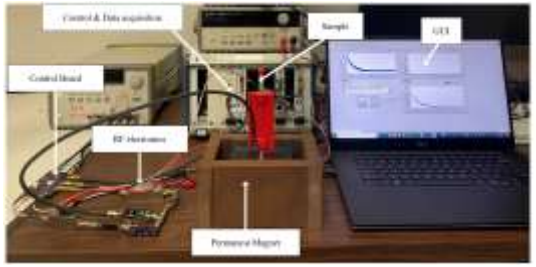
Collogue asks if it can be done?

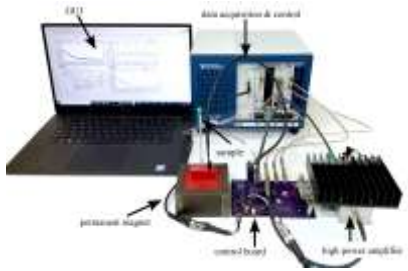
Tracking down specialized hardware, magnets cost 10-20k

Coil magnet design







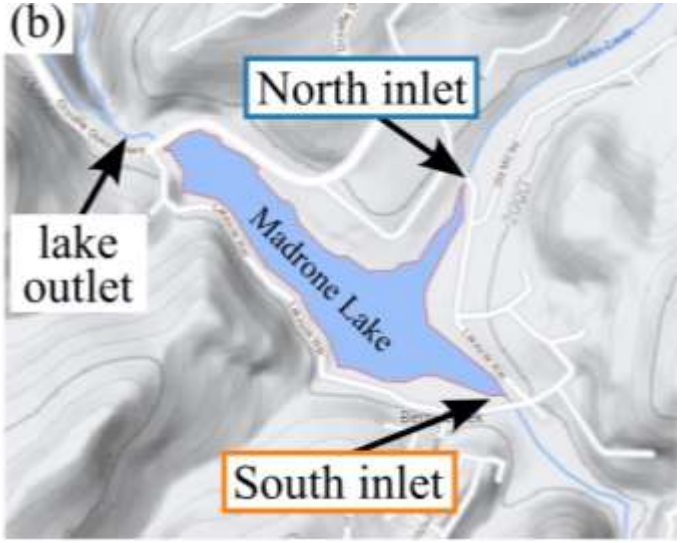


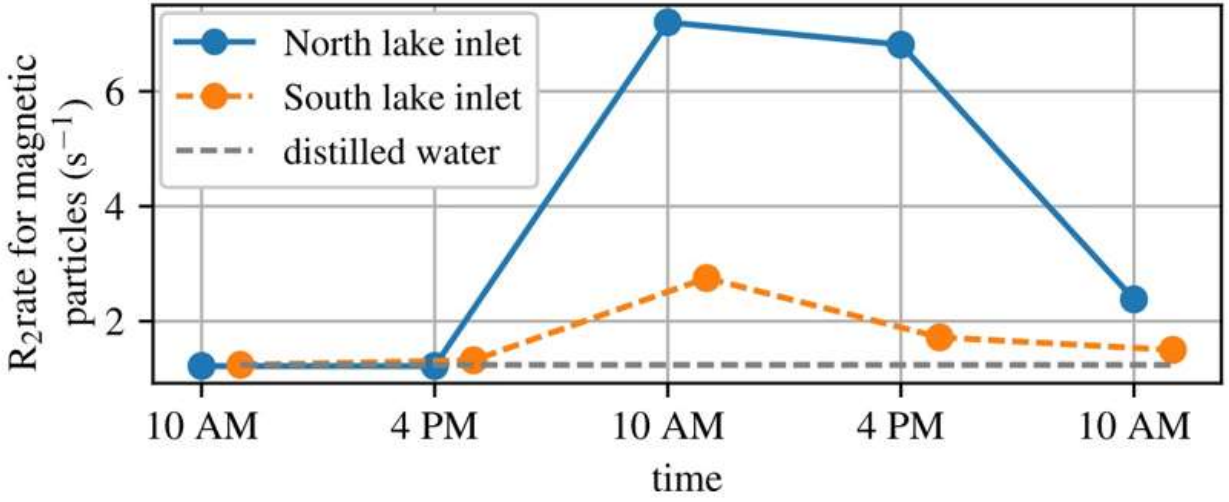
Open-source Design

Continuous Water Quality Monitoring

The system is being developed to:

- Track T2 relaxation over time
- Use AI/ML to infer contaminants
- Report results via web portal
- Integrate into a larger autonomous monitoring framework
- Enable continuous surveillance

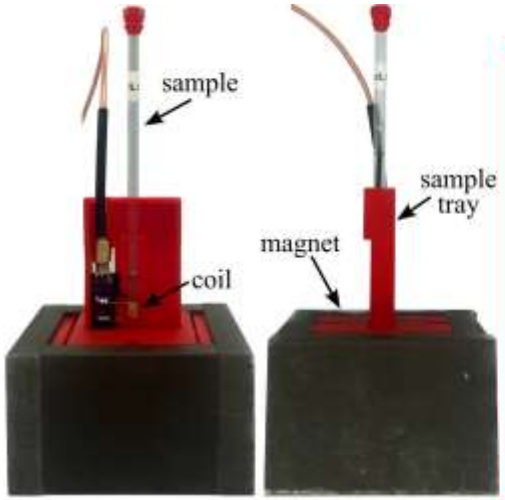


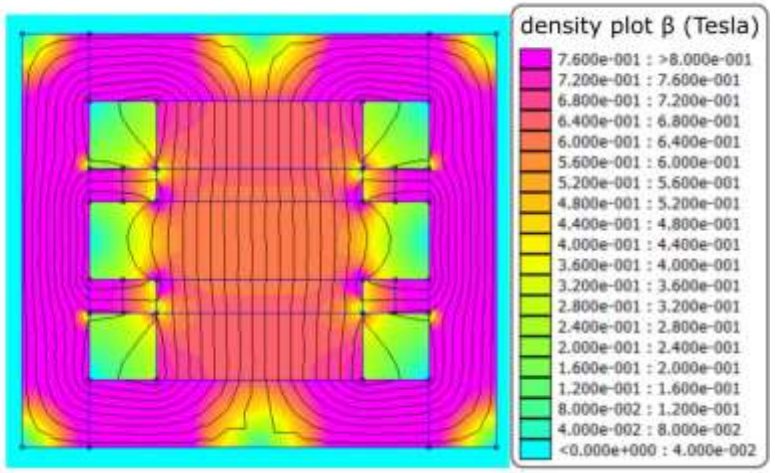


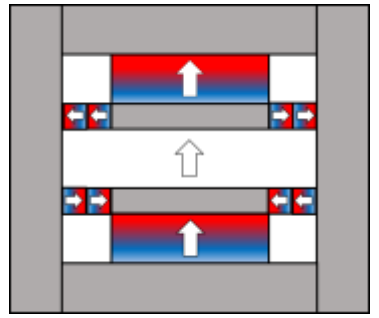
Open-source NMR Hardware

Permanent Magnet Array

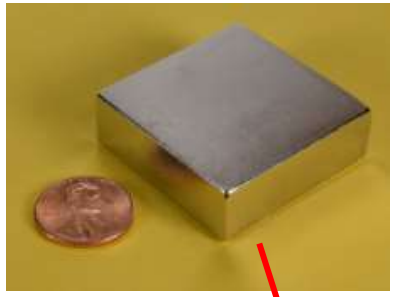
- **0.565 T** strength at 23ºC
  - -800 ppm/K gradient
- Larmor (operating) frequency:
  - $f_{Larmor} = \gamma B = \left(42.58 \frac{MHz}{T}\right)(0.565\ T) \approx \mathbf{24\ MHz}$
- 150 ppm homogeneity
- 4.4 lbs



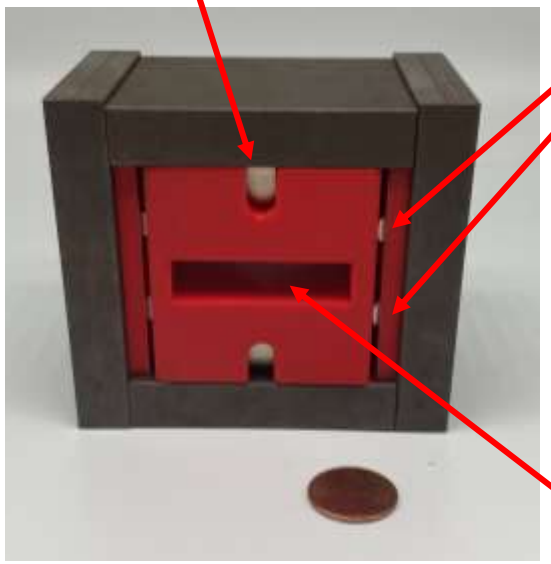




N42 magnet



N42 magnet



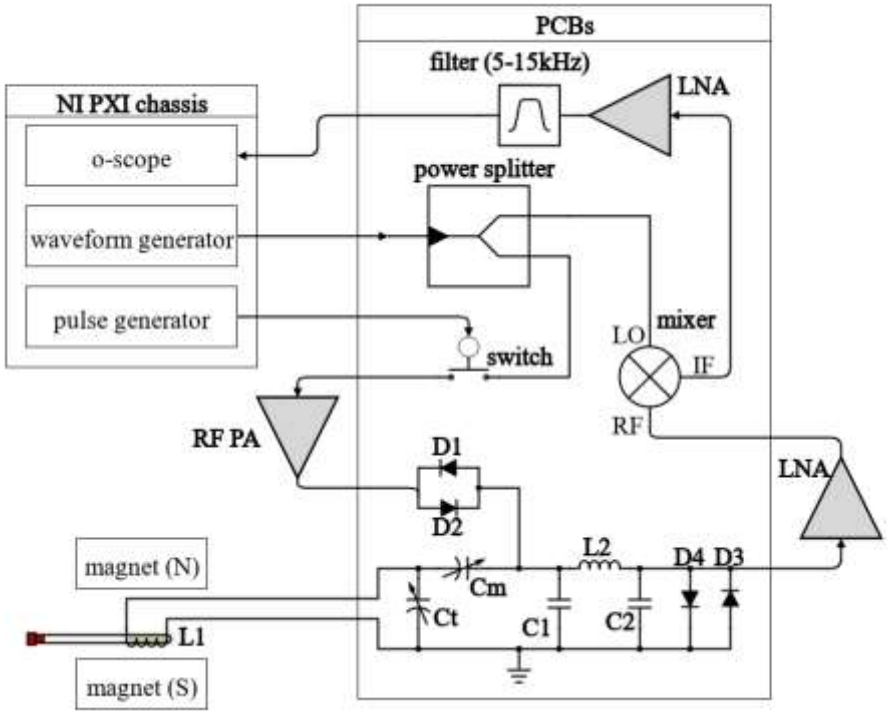
Sample location

Fully assembled

RF Electronics

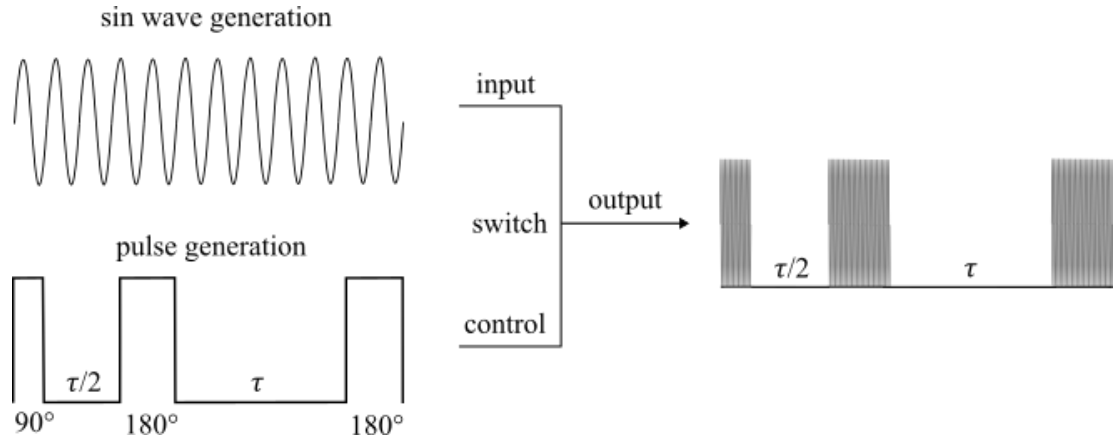
- A single 24 V DC power supply required
- Impedance of all cables and PCB traces matched to 50 Ω
- Waveform generator → sine wave at Larmor frequency
- Pulse generator → follows CPMG pulse train
- Duplexer (crossed diodes) isolates probe and LNA

General flow

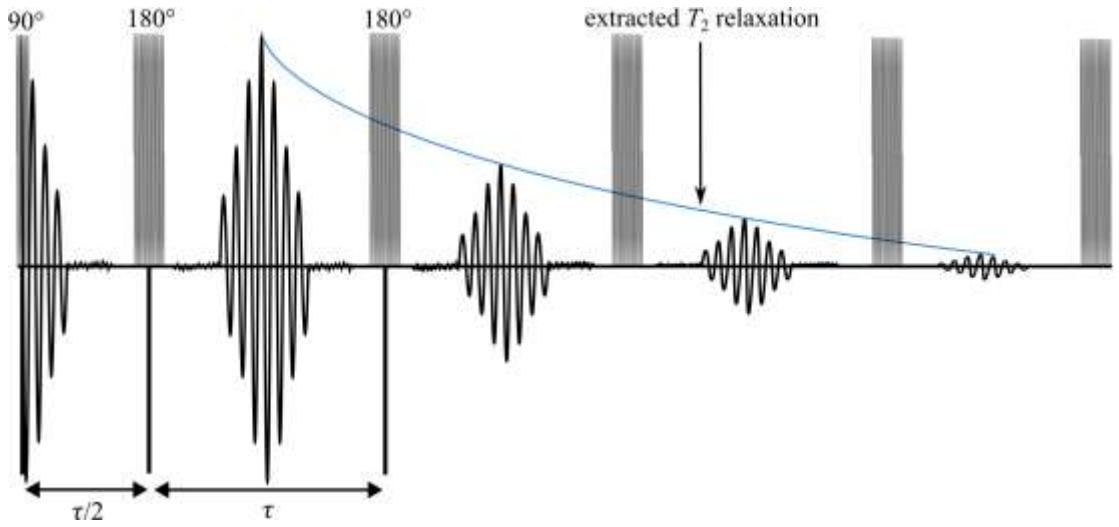


Signal Generation and Control

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

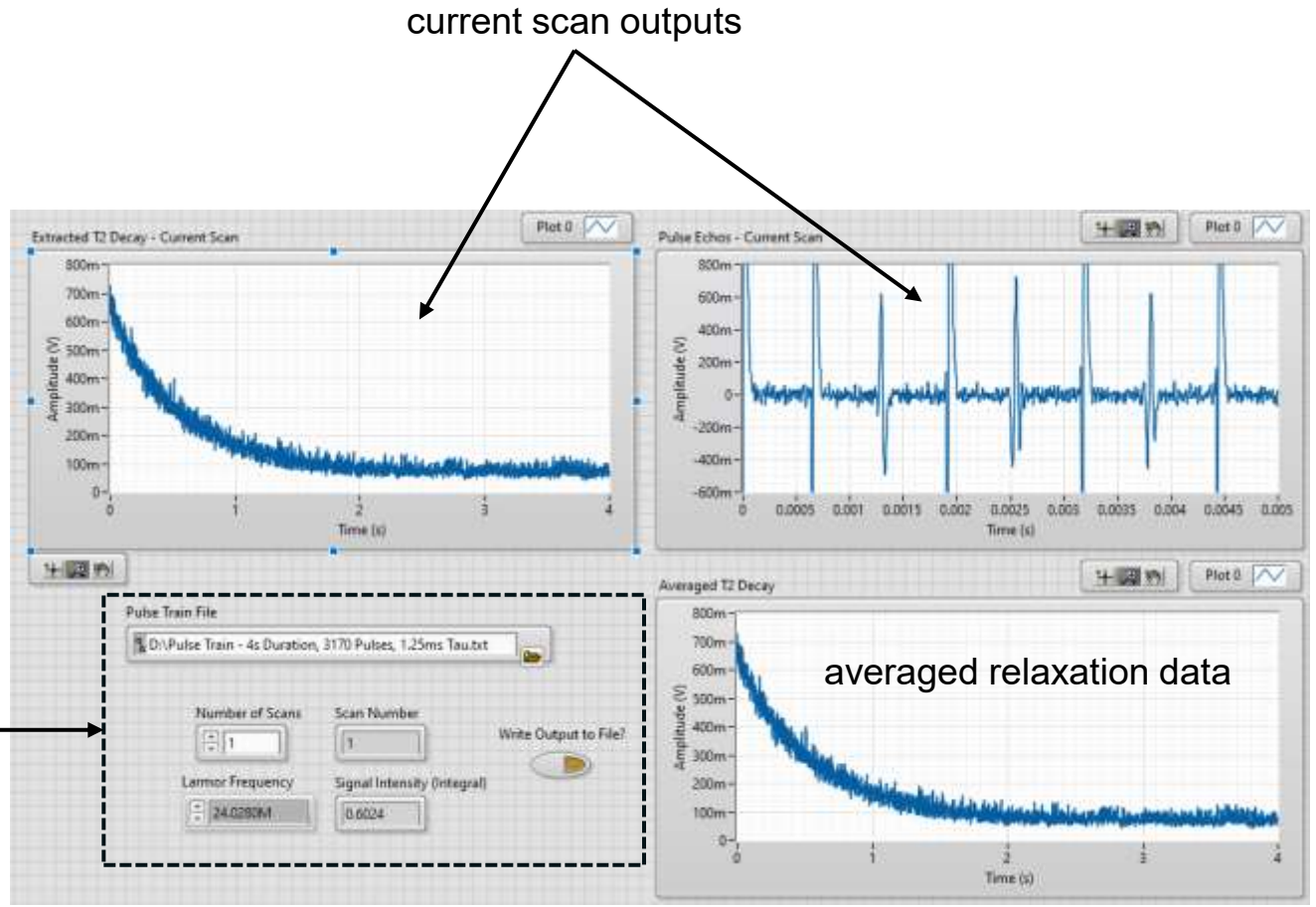


- Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence
  - $90°$ pulse duration is 7 μs
  - $\tau = 1.25$ ms



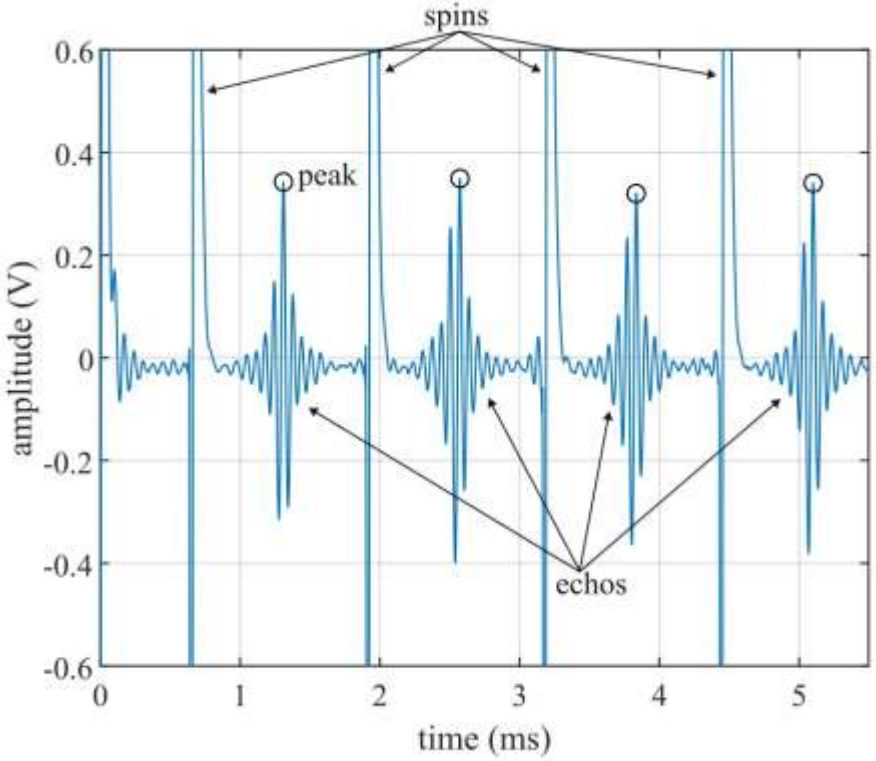
Data Acquisition

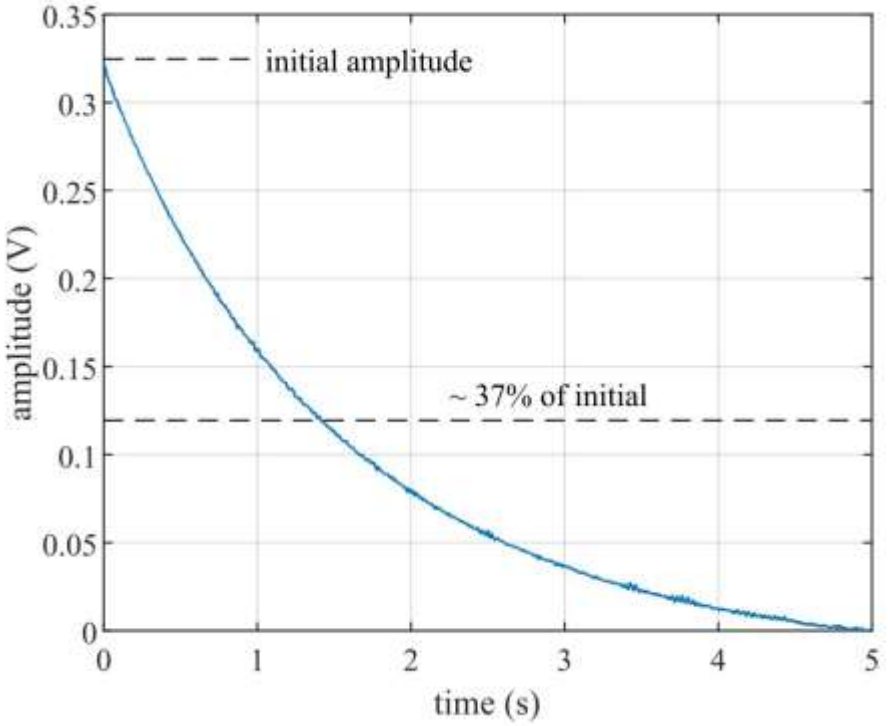
- LabVIEW GUI serves as front end
- Each test comprises 5 scans (averages)
- Time for T_2 curve acquisition < 10 seconds
- Thermocouple used for frequency calibration



TD-NMR Signals and MP Content

- 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 MP concentration well established

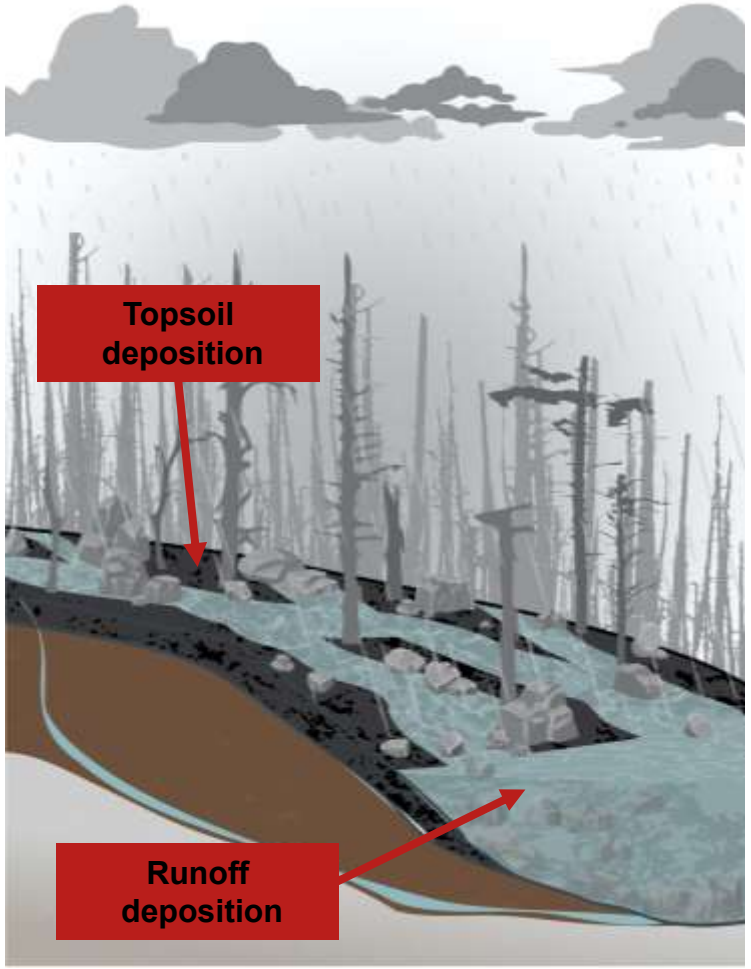




Use Case: Wildfire Ash

Why Monitor Magnetic Contents of Wildfire Ash?

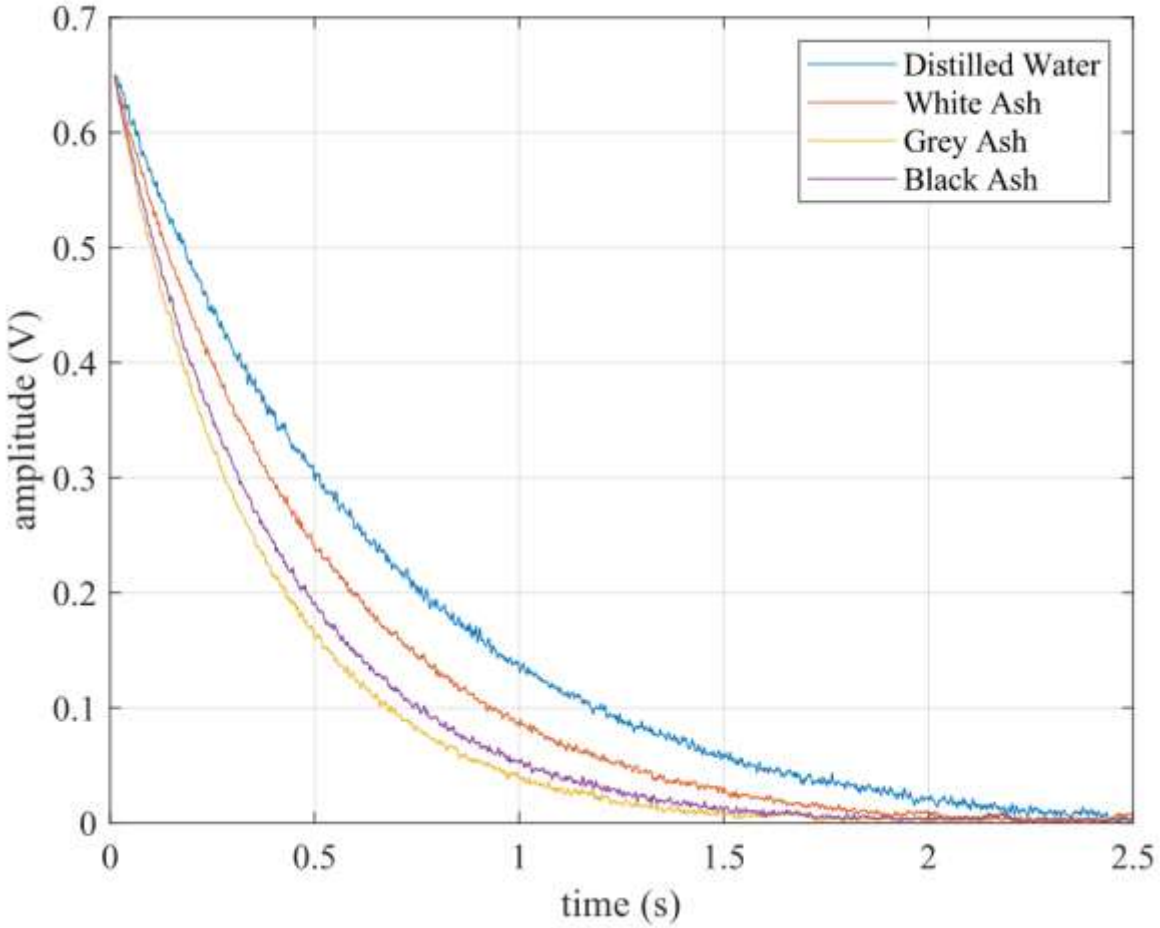
- Effects on topsoil
  - Ash deposits enhance magnetic content in soil
  - Magnetic properties are closely related to climate & rainfall
- Deposition through runoff water
  - Nearby bodies of water accumulate magnetic content
  - Nanoscale magnetite is linked to brain disease
- Understand fire severity and the reaches of magnetic deposition



USGS, "How wildfires threaten U.S. water supplies," Water Data Labs, 06-Nov-2020. [Online]. Available: https://labs.waterdata.usgs.gov/visualizations/fire-hydro/index.html#/. [Accessed: 28-Oct-2022].

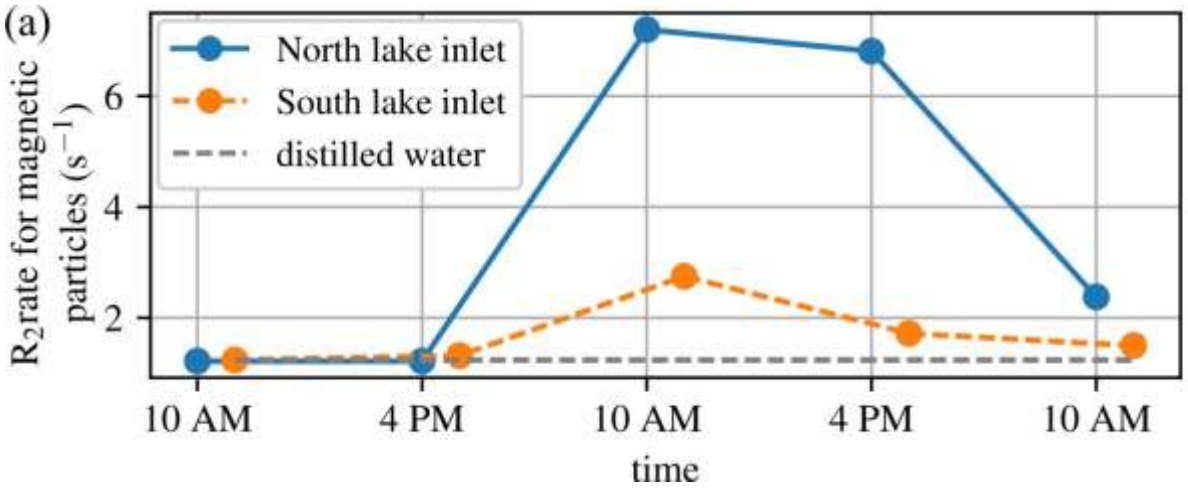
NMR Relaxometry with MPs

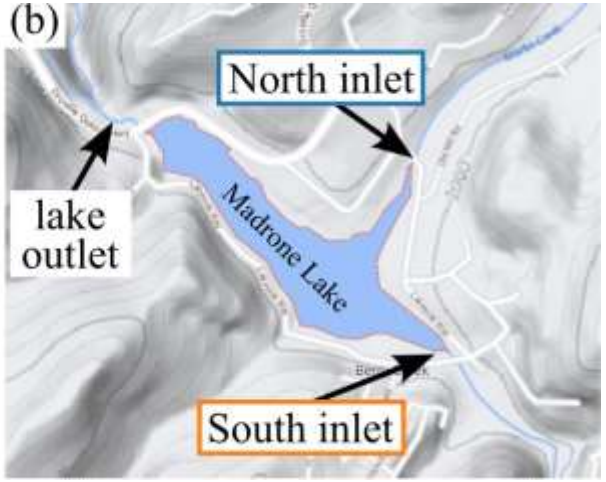
- 10 total ash samples
- 20 mg in 20 mL of water
- Distilled water used as reference
- R_2 extracted via least squares regression
  - $M_{xy} = M_0 \exp(-R_2 t)$



Real-time In Situ Tracking

- Monitoring Wildland-Urban Interface Fire Ashes and Run off Total iron content collected
- 10 surface water samples collected from two inlets to Lake Madrone that were subjected to runoff following the North Complex Fire in California





ML-based Species Parameter Classification

Patent Pending

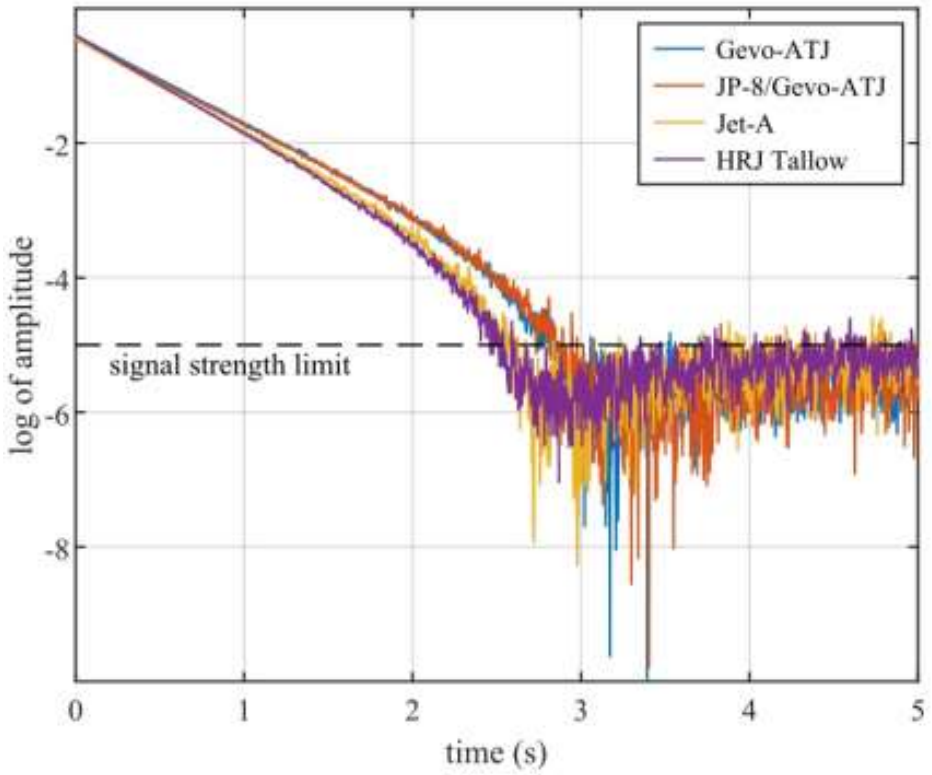
Background: Predicting DCN of Jet Fuel

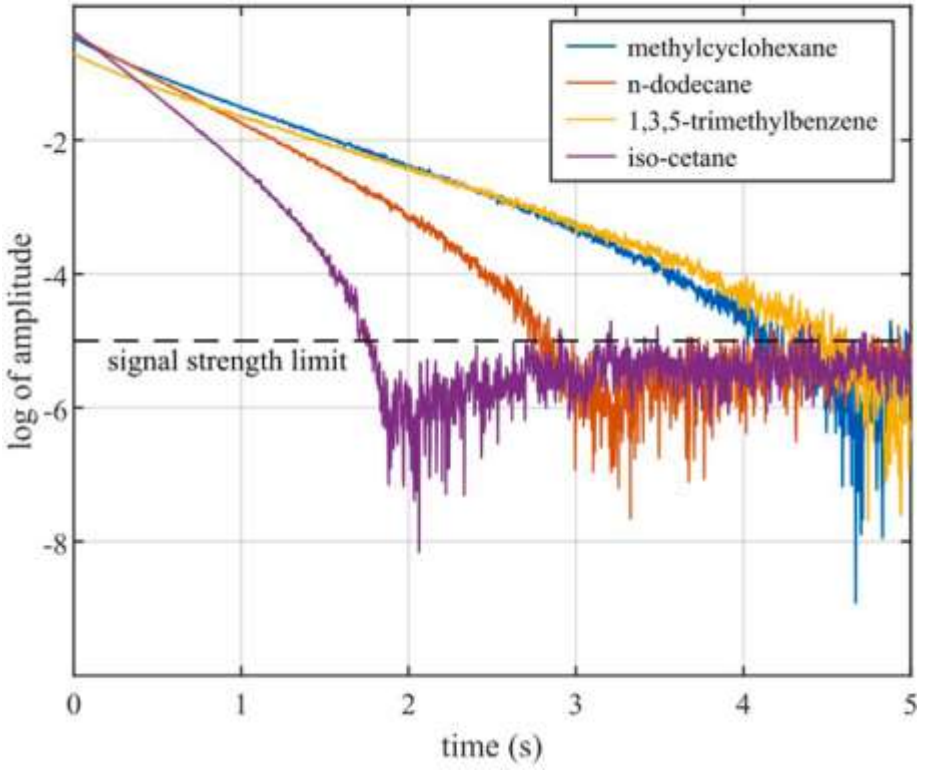
- The Derived Cetane Number (DCN) is a widely used metric that indicates a fuel's ignition quality and combustion behavior.
- Higher DCN typically means better ignition propensity and more efficient combustion, which directly impacts engine performance and emissions.
- Traditional DCN measurement methods (e.g., ASTM standards) require large-scale, time-consuming lab tests.

Jelson25, Public domain, via Wikimedia Commons

Separating Signal from Noise

- Natural logarithm of T2 signal allows for the separation of signal and nose



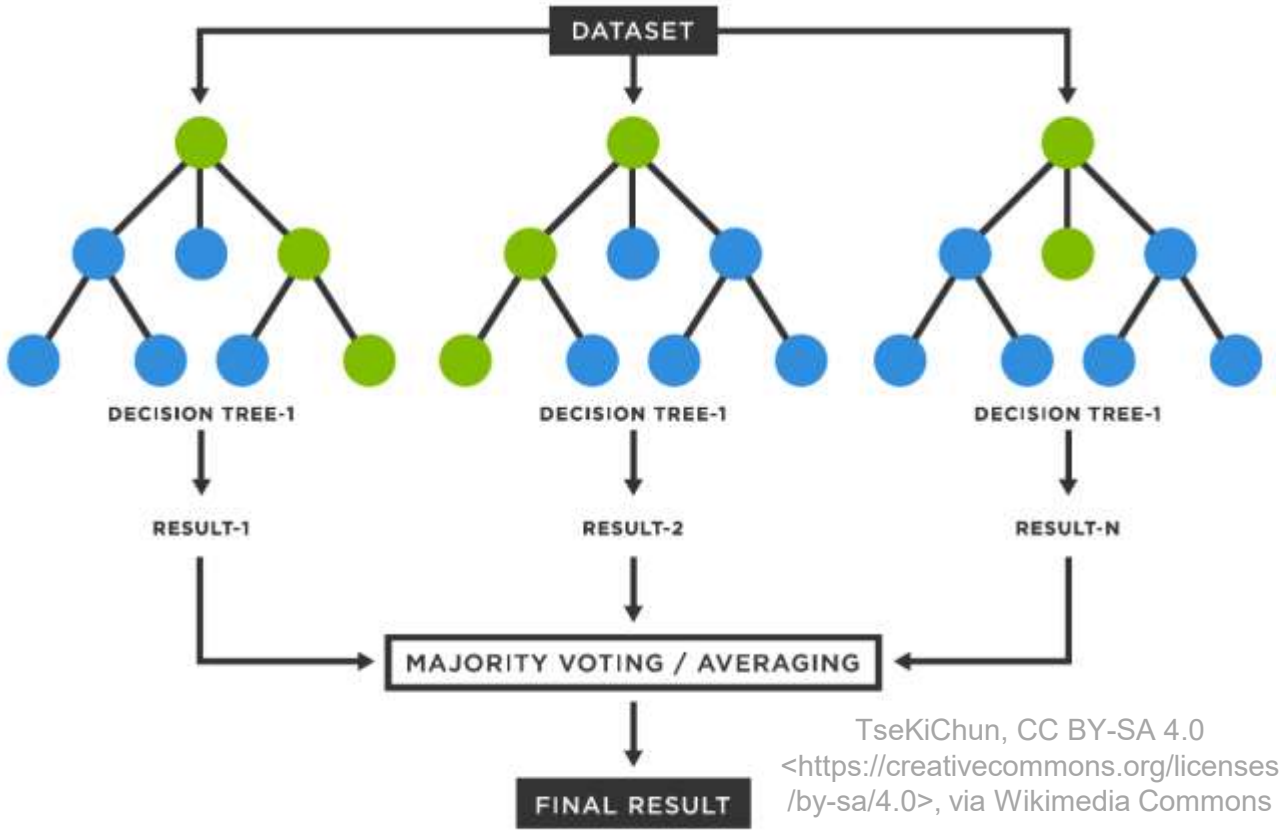


Patent Pending

Feature-based Classification using Interpretable Machine Learning

- Visual summary of the interpretable machine learning approach.

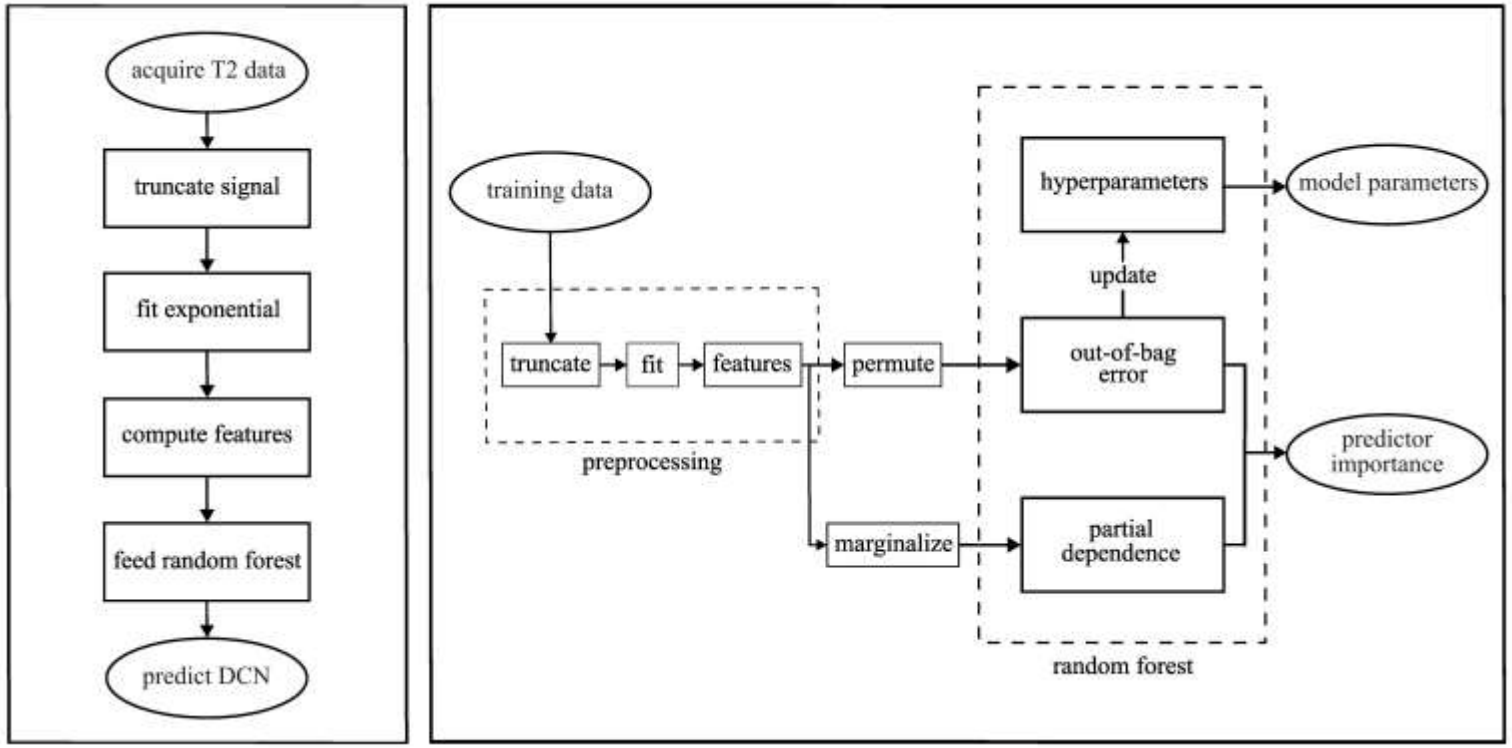
feature	interpretation	formula
amplitude	initial signal strength	x_a
rate	T_2 relaxation rate	x_b
mean	average value	$\frac{1}{N}\sum_{i=1}^{N} x_i$
standard deviation	spread around the mean	$\sqrt{\frac{\sum_{i=1}^{N}(x_i-\bar{x})^2}{N}}$
root mean square	average power	$\sqrt{\frac{1}{N}\sum_{i=1}^{N} x_i^2}$
shape factor	signal shape	$\frac{x_{rms}}{x_{mean}}$
kurtosis	tail length	$\frac{\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^4}{[\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^2]^2}$
skewness	signal asymmetry	$\frac{\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^3}{[\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^2]^{3/2}}$
impulse factor	ratio of amplitude to mean	$\frac{x_a}{x_{mean}}$
crest factor	ratio of amplitude to RMS	$\frac{x_a}{x_{rms}}$



Patent Pending

Interpretable Machine Learning

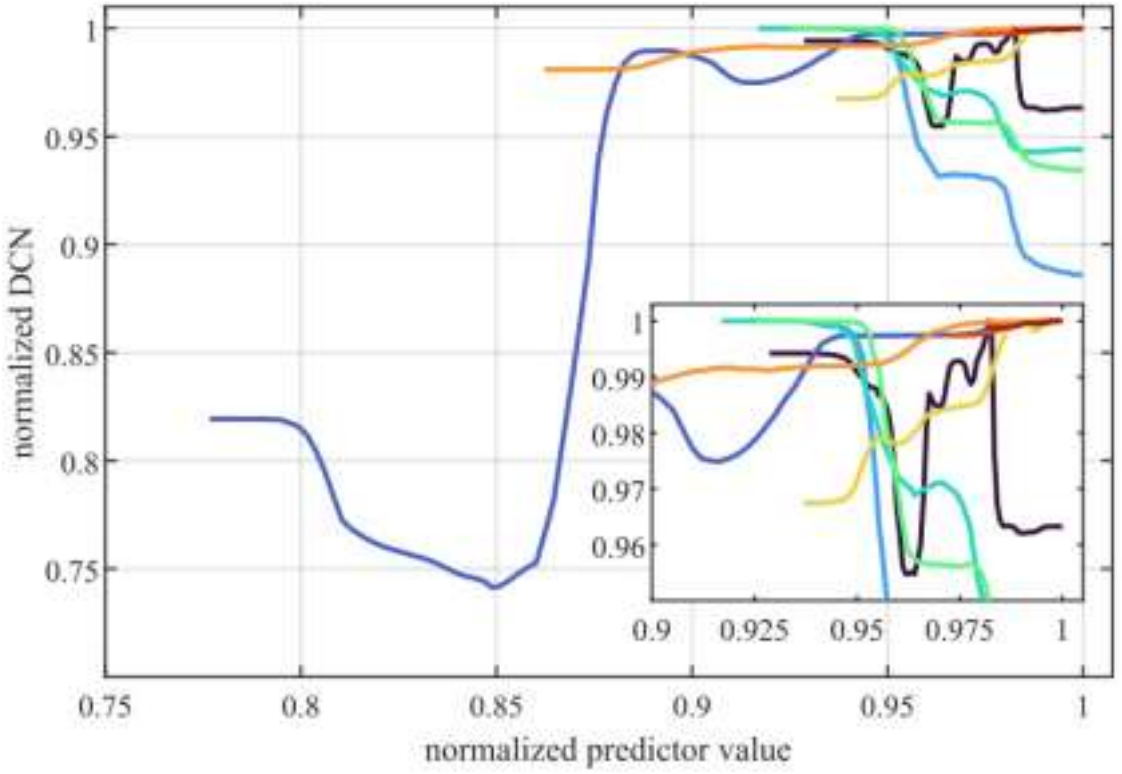
- A random forest model is trained with hyperparameter tuning, generating feature importance scores that highlight which input variables most influence the prediction of DCN.



Patent Pending

Partial Dependence Plots

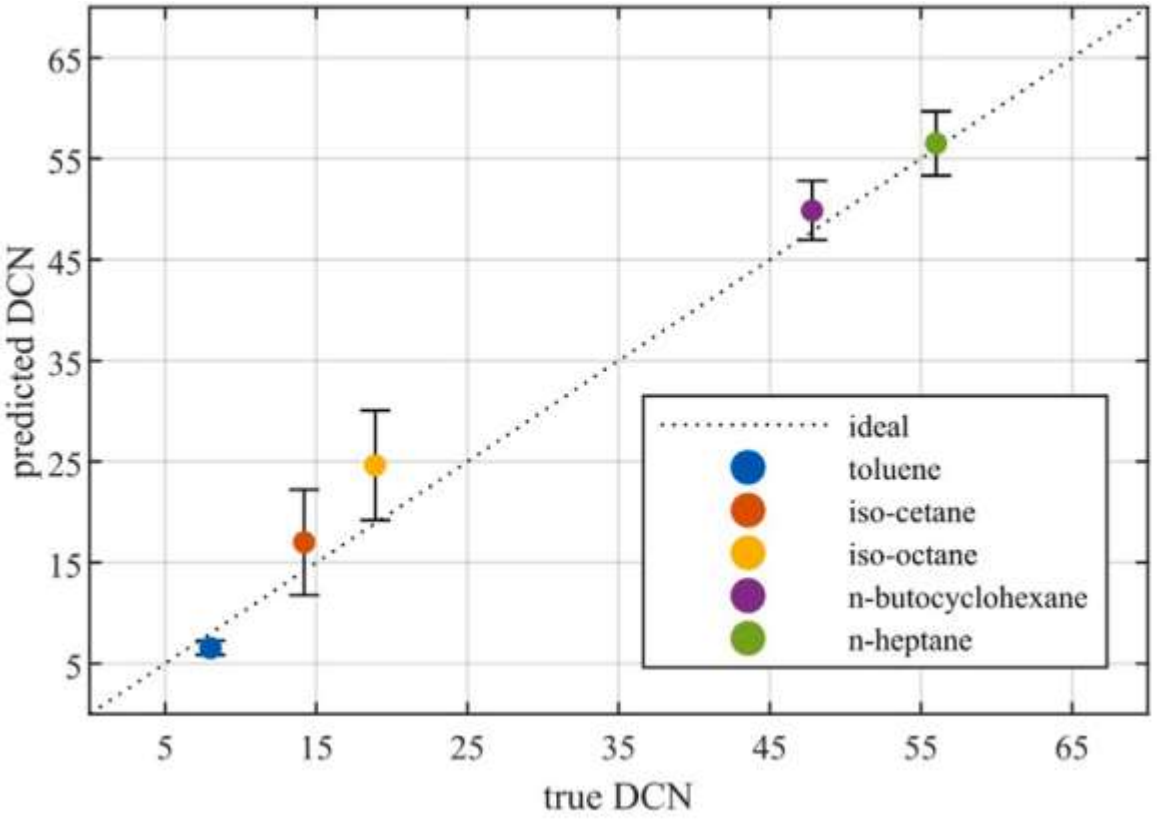
- Partial dependence plots (PDPs) are a powerful tool used in machine learning and statistical analysis to interpret the relationship between a set of features (variables) and the predicted outcome of a model.



Patent Pending

ML-based DCN Prediction

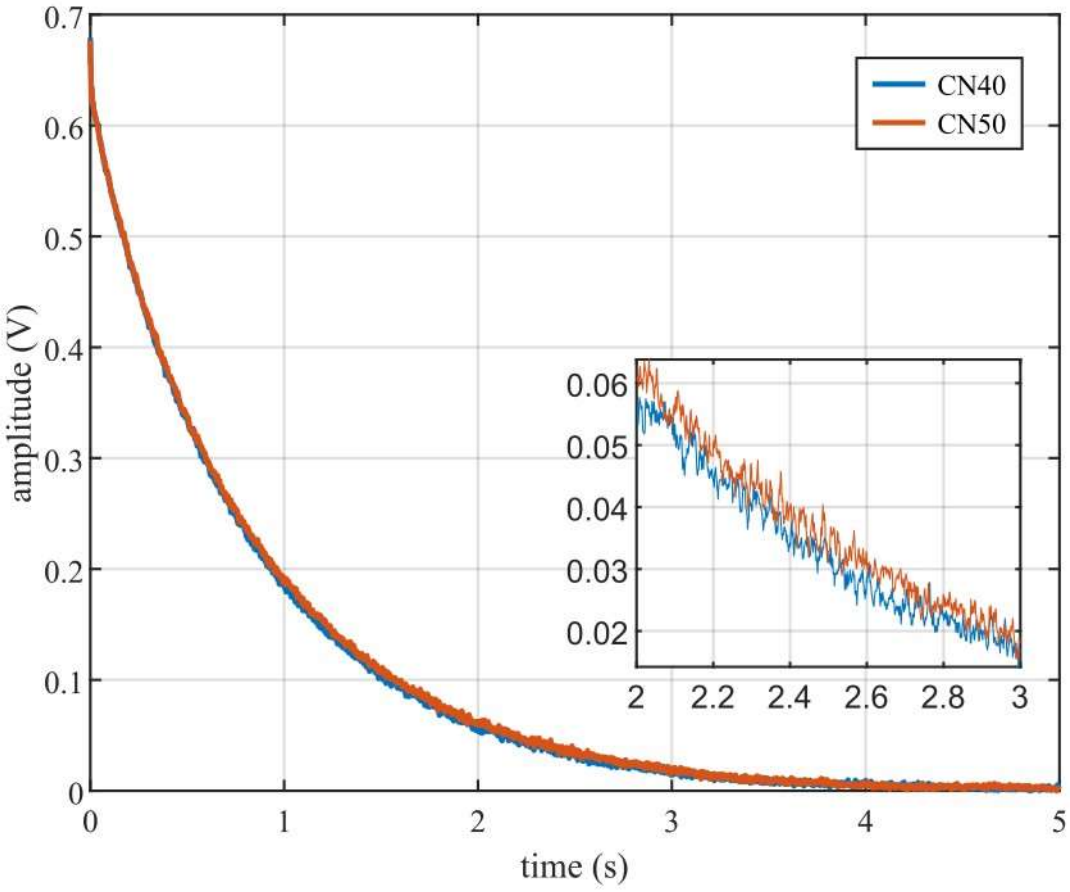
- Model predictions for pure hydrocarbons show strong accuracy.
- Validation dataset results closely match true DCN values.
- Standard deviation (error bars) indicate minimal variation.
- Demonstrates the reliability of the approach for well-characterized fuels.



Patent Pending

Distinguishing Similar T_2 Curves

- The interpretable ML approach accurately infers DCN from T_2 relaxation curves.
- CN40 and CN50 were used as test samples and were not included in training.
- The relaxation curves of CN40 and CN50 appear visually similar.
- Computed features from their T_2 curves differ by less than one part per hundred.

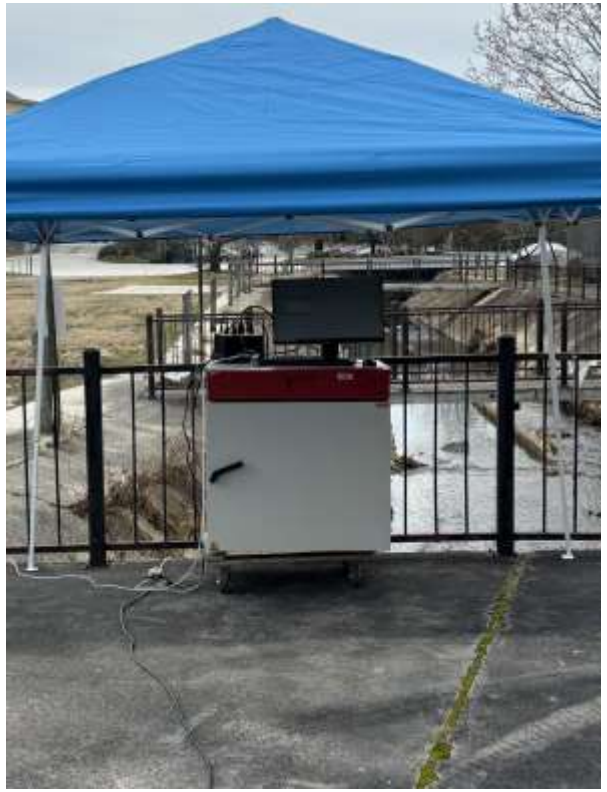


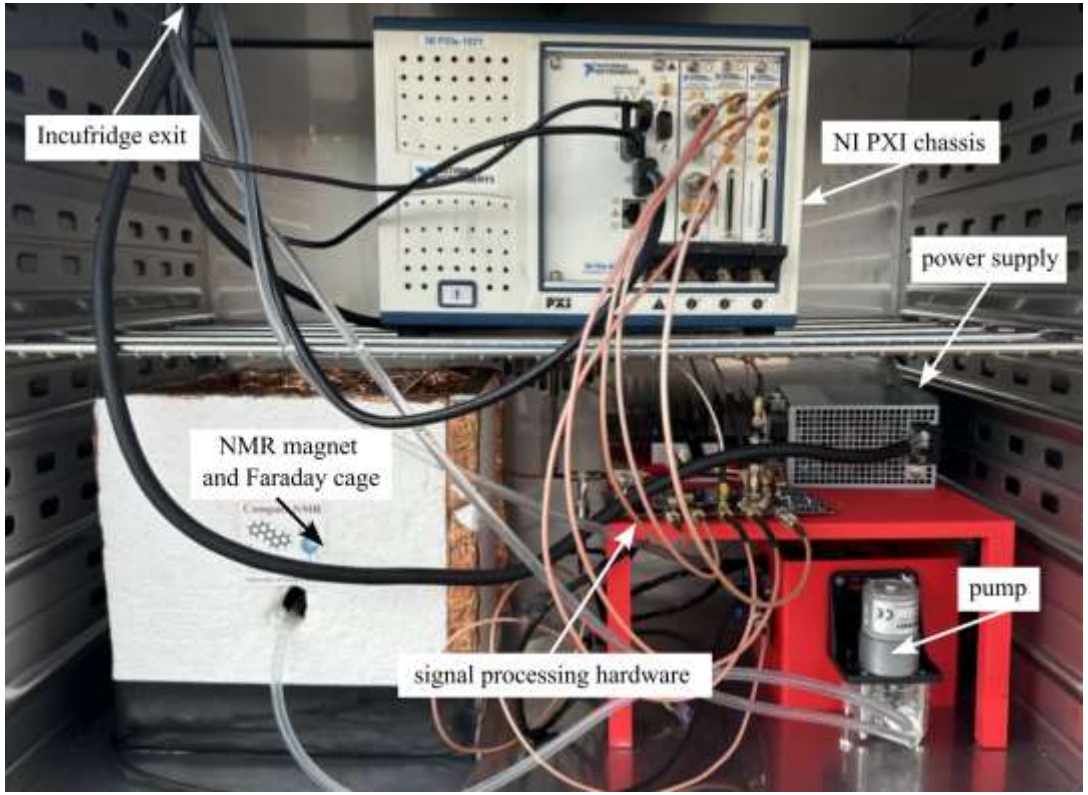
Patent Pending

Ongoing In Situ Monitoring Work (Preliminary Testing)

Preliminary NMR Deployment

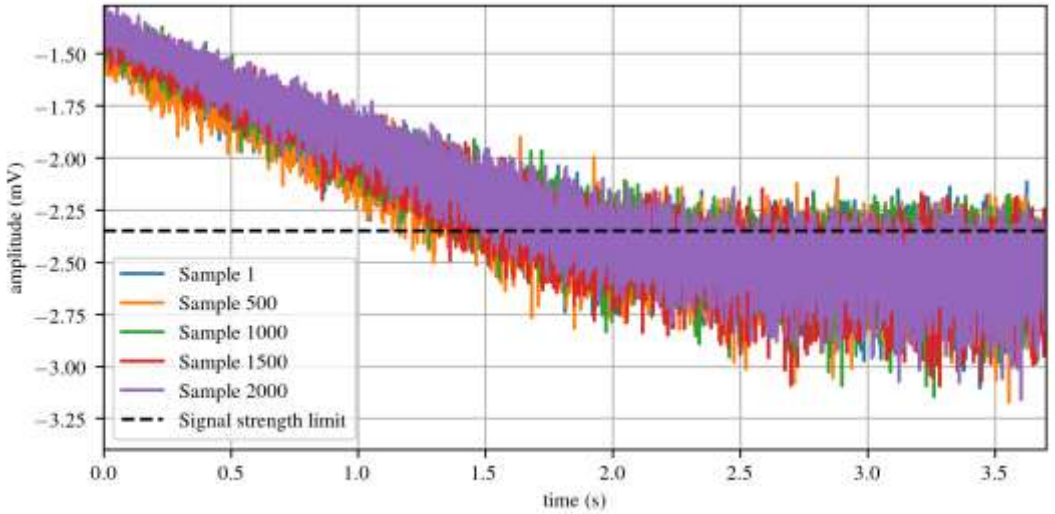
- Initial field deployments in Columbia South Carolina

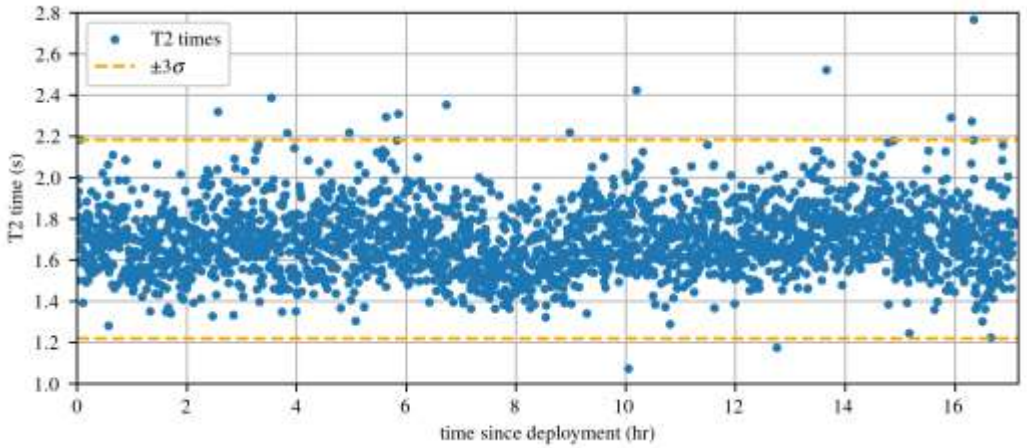




Preliminary T2 Results

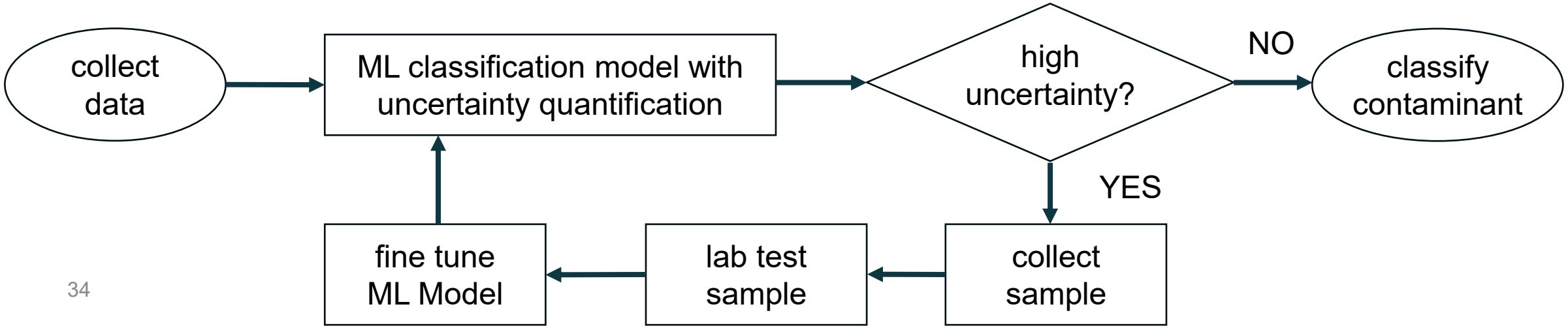
- T_2 data was tracked over 17 hours and remained mostly stable, as expected.
- No averaging was applied, resulting in a slightly noisy signal.
- Future work will involve:
  - Deploying during a rainstorm to continuously track runoff changes.
  - Collecting detailed water samples for further analysis.
  - Training the interpretable ML model on extracted water features.





Future Work: Fine-tuning ML Model

- The flow-through NMR will be deployed with an automatic water sampler and will trigger a sample based on uncertainties in predicted contaminate.
  - Collected samples will be returned to the lab for further assessment.
  - Lab results will be used to fine-tune the model
  - Over time, fewer lab samples will be required as the AI/ML model will more closely track the system.
  - Unknown contaminates events will trigger sample be taken, limiting False Negatives.



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Thank You for Your Time

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