Field Deployable NMR for In Situ Water Quality Monitoring

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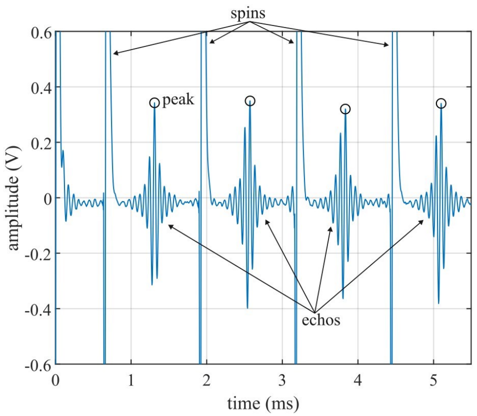
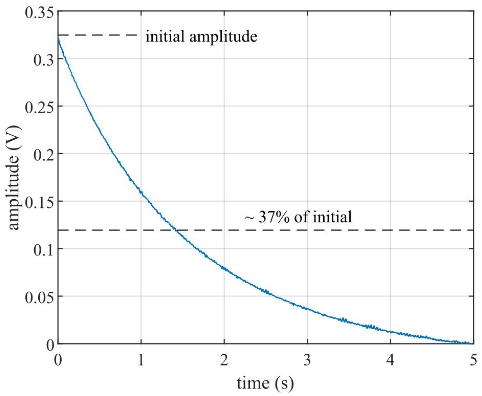
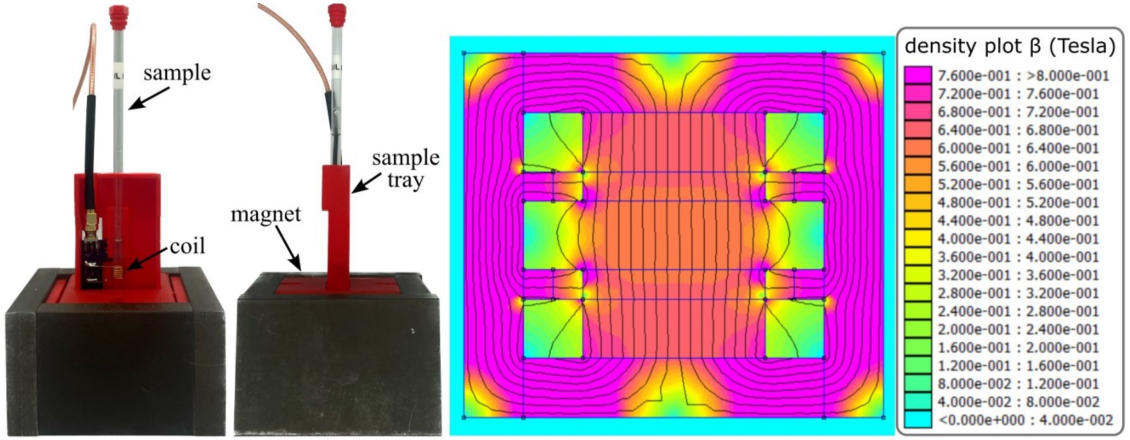
Outline for Today's Talk

- NMR Basics
- Our Open-source NMR System
- Use Case: Wildfire Ash
- Lab Data Collection for Model Training
- Field Deployment of In Situ NMR system

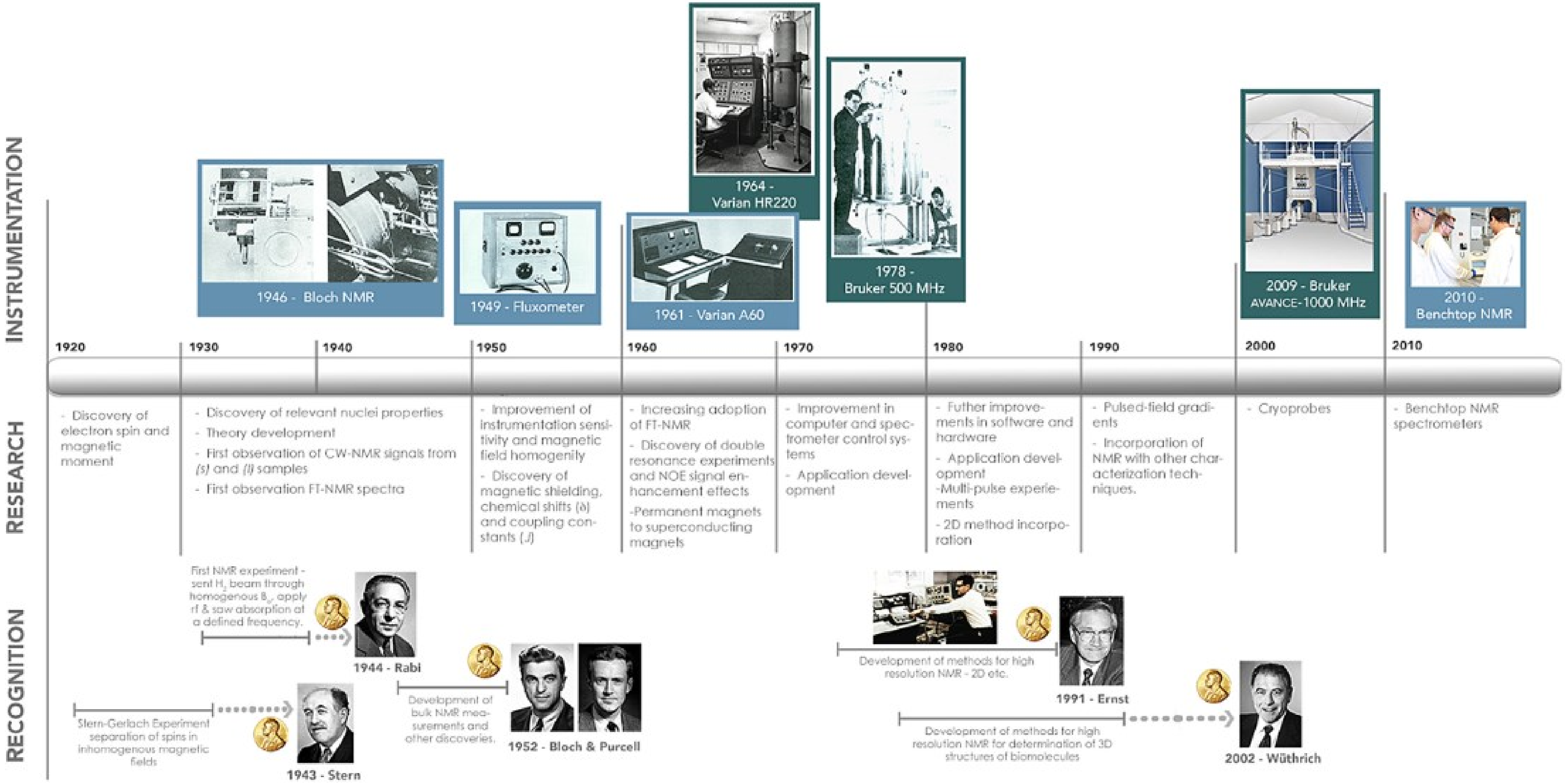






NMR Basics

History of NMR

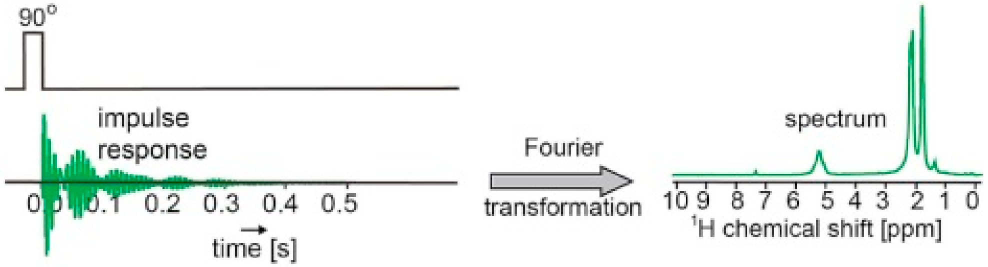


Riegel, Susanne D., and Garett M. Leskowitz. "Benchtop NMR spectrometers in academic teaching." TrAC Trends in Analytical Chemistry 83 (2016): 27-38.

Nuclear Magnetic Resonance (NMR) Techniques

NMR spectroscopy

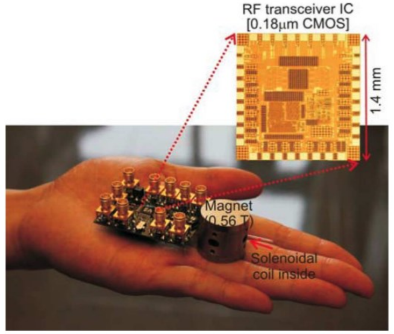
- Lab-Grade NMR
  - Frequency domain analysis
  - High resolution
  - Expensive & bulky

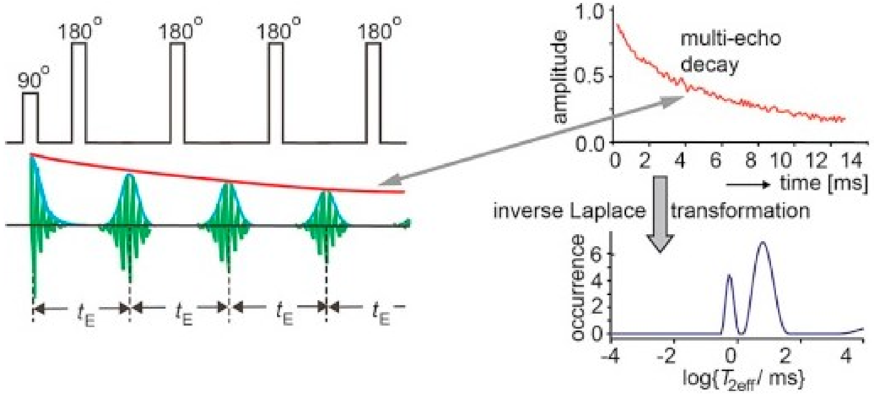


B. Blümich, “Introduction to compact NMR: A review of methods,” TrAC Trends in Analytical Chemistry, vol. 83, pp. 2–11, Oct. 2016.

NMR Relaxometry

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





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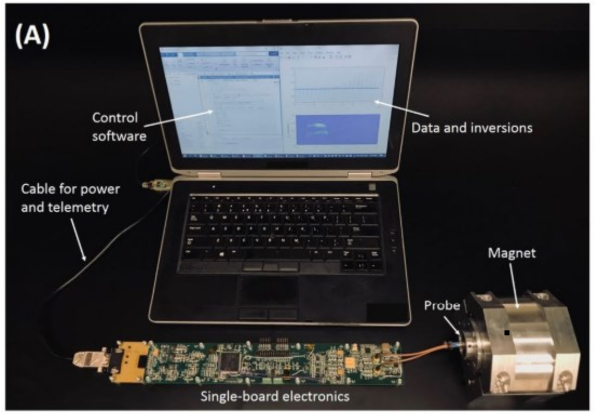
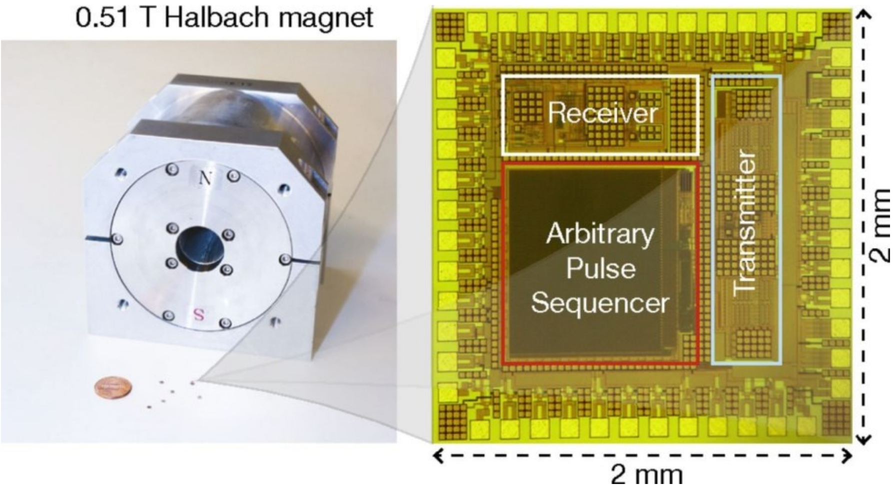
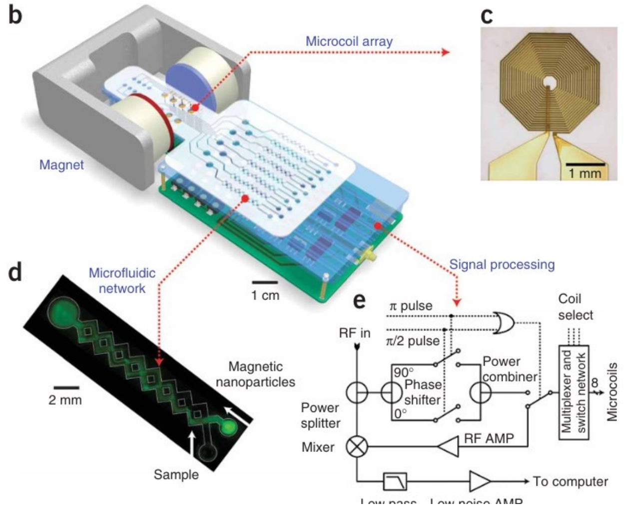
Miniature NMR systems



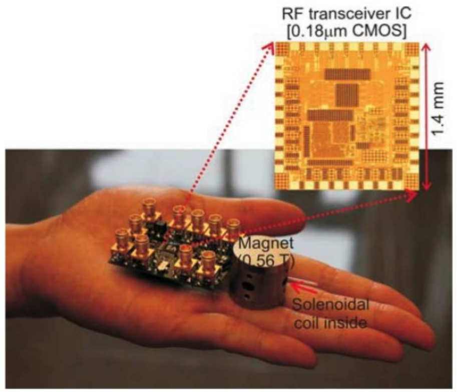
Tang, Yiqiao, David McCowan, and Yi-Qiao Song. "A miniaturized spectrometer for NMR relaxometry under extreme conditions." Scientific reports 9.1 (2019): 11174

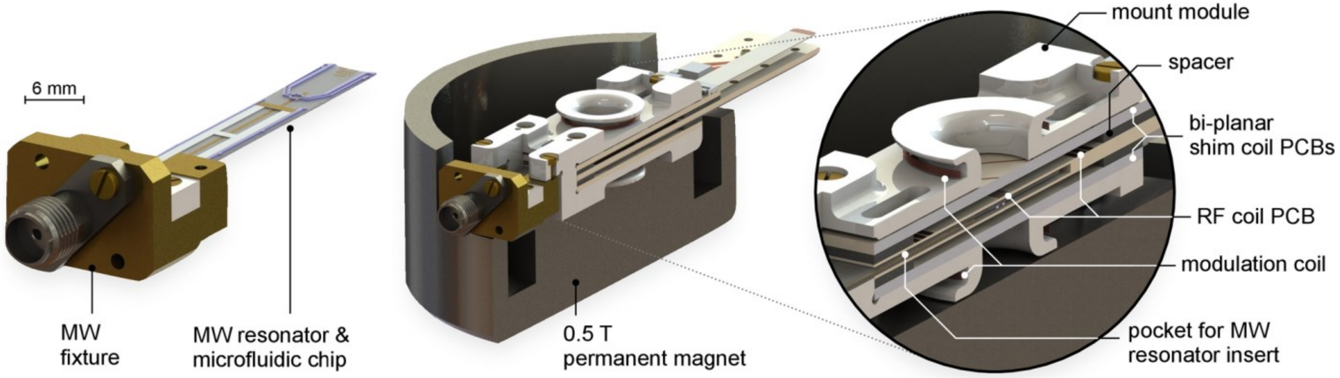


https://physicsworld.com/a/going-mobile-with-nmr-spectroscopy/



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





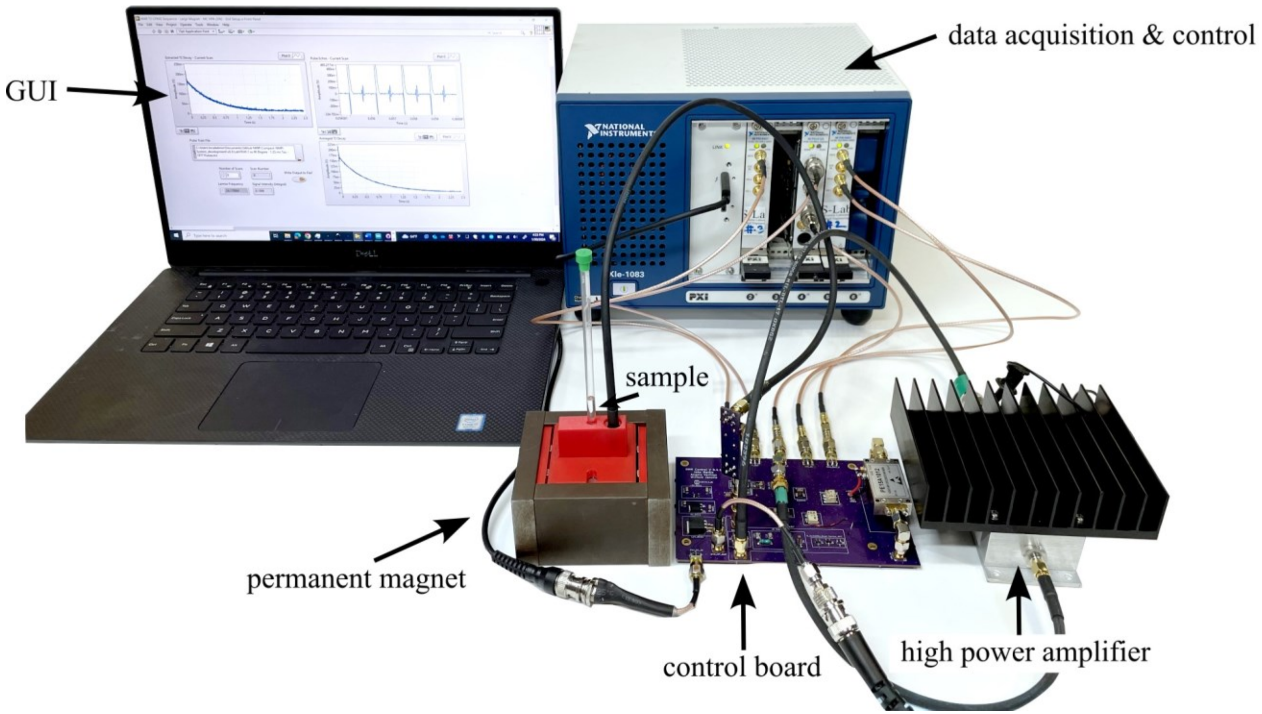
Sun, Nan, et al. "Palm NMR and 1-chip NMR." *IEEE Journal of Solid-State Circuits* 46.1 (2010): 342-352.

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

- Hardware and Software shared through a public repository
- A paper published in HardwareX to assist in building sensor
- Cost is approximantly $2,000 + DAQ system



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Hardware article

Open-source compact time-domain hydrogen (1H) NMR System for Field Deployment

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ABSTRACT

This paper presents a compact, low-cost time-domain nuclear magnetic resonance (TD-NMR) system based on a 0.5 T permanent magnet designed for in-situ ^{1}H measurements. Unlike conventional high-field nuclear magnetic resonance (NMR) spectrometers, this system emphasizes relaxation times rather than chemical shifts, enabling material property analysis without large magnets or complex spectral processing. The hardware employs an off-the-shelf data acquisition and control system along with a custom PCB for signal conditioning, ensuring straightforward deployment and reduced costs. The system's core sequence is a Carr-Purcell-Meiboom-Gill pulse train, chosen for efficient T_2 relaxation measurements under varying magnetic susceptibilities. By focusing on relaxation measurements, this approach bypasses complexities of high-resolution spectroscopy, enhances signal-to-noise in low-field conditions, and enables robust characterization across challenging environmental settings. We validate the system using aqueous Copper(II) sulfate solutions, correlating T_2 values with copper concentrations to simulate environmental heavy metal contamination monitoring. Prior work has demonstrated versatility in fuel property analysis and environmental sensing, confirming broad applicability for this portable platform. While packaging and integration with ancillary equipment (e.g., flow-through systems) are not covered, the platform serves as a versatile foundation for specialized deployments. Its open-source design and affordability aim to democratize NMR technology and extending its utility beyond conventional laboratory environments. This accessible configuration fosters widespread educational and professional use.

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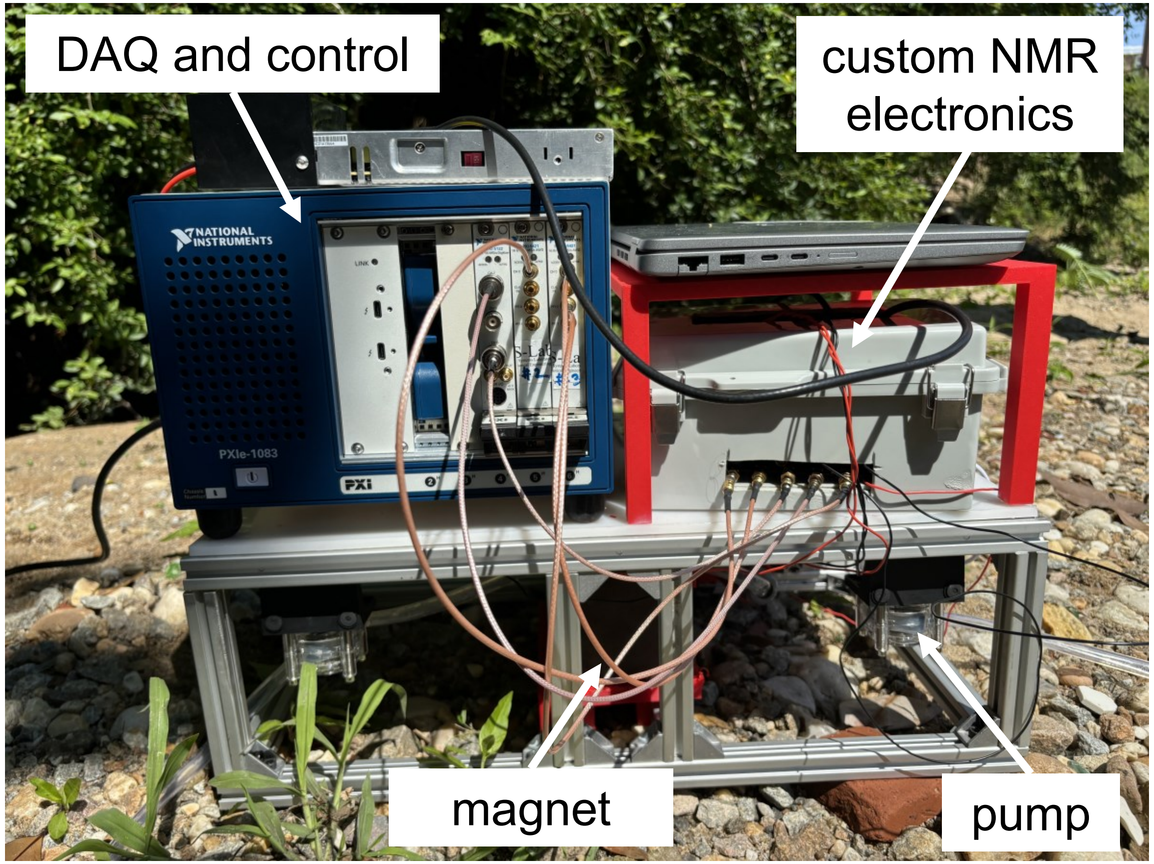
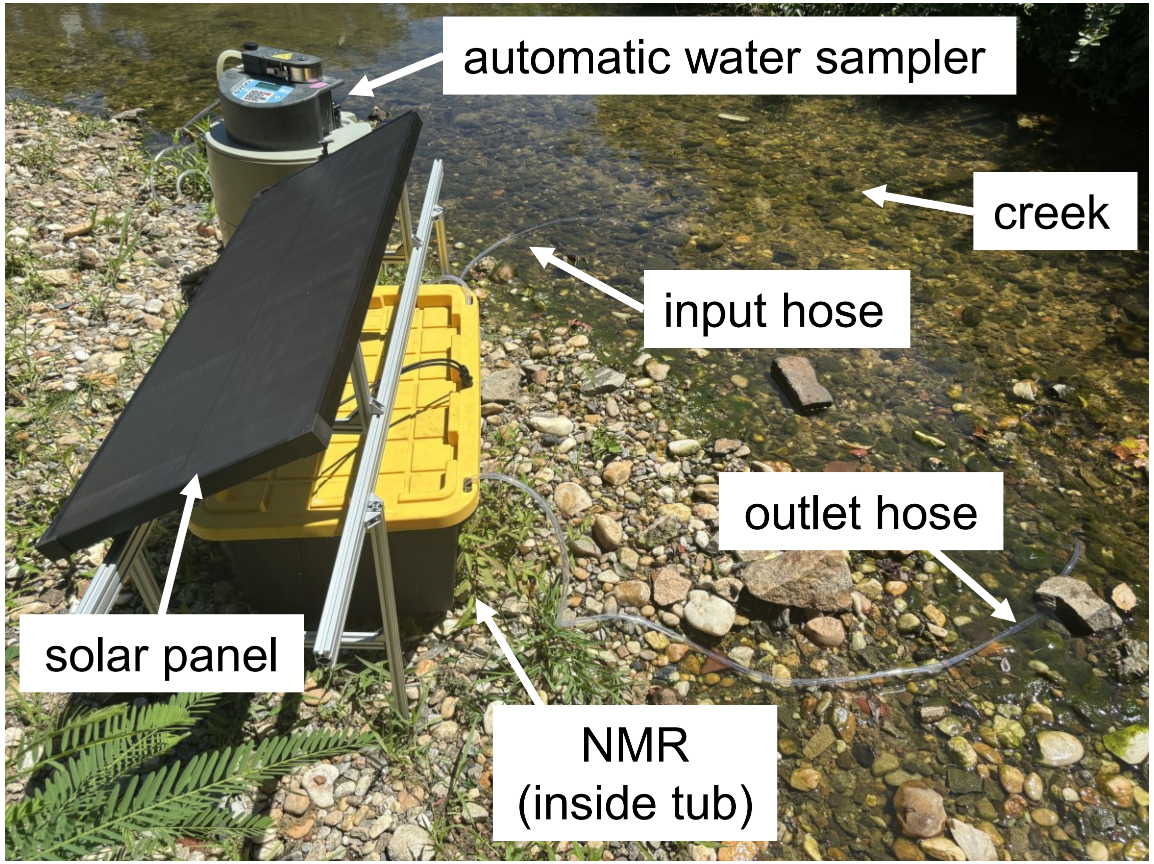
Winford Janvrin, Jacob Martin, Daniel Hancock, Angelo Varillas, Austin R.J. Downey, Perry J. Pellechia, Joud Satme, and Sang Hee Won. Open-source compact time-domain hydrogen (1H) NMR system for field deployment. HardwareX, 22:e00651, June 2025. doi:10.1016/j.ohx.2025.e00651

Flow-through NMR





Past NMR Development

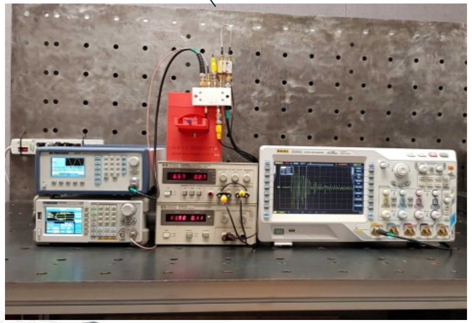
2019 | 2020 | 2021 | 2022 | 2023 | 2024 | 2025

Funding: Downey/San Hee | Army | USC | NSF CA

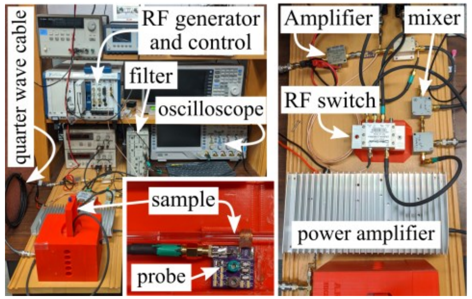
Hardware

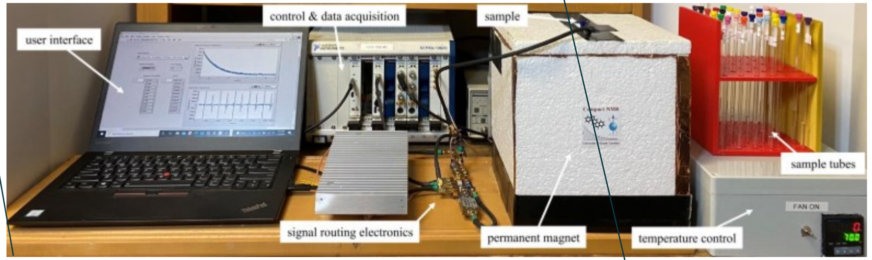
Collogue asks if it can be done?

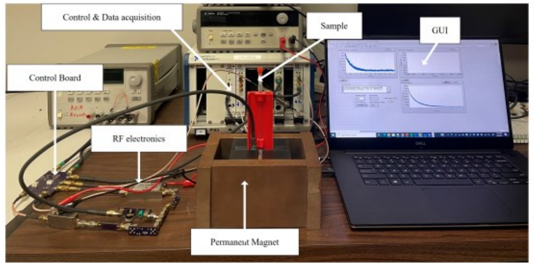
Tracking down specialized hardware, magnets cost 10-20k

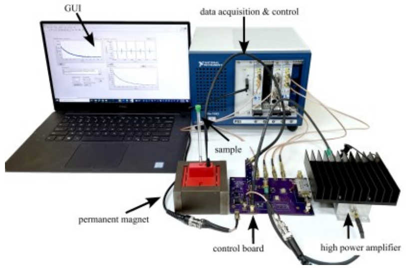


Coil magnet design







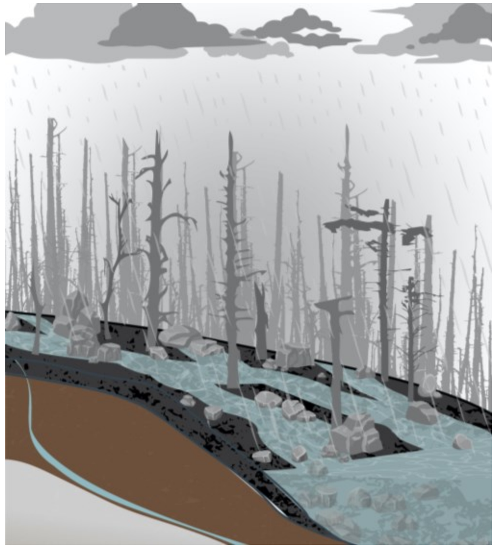


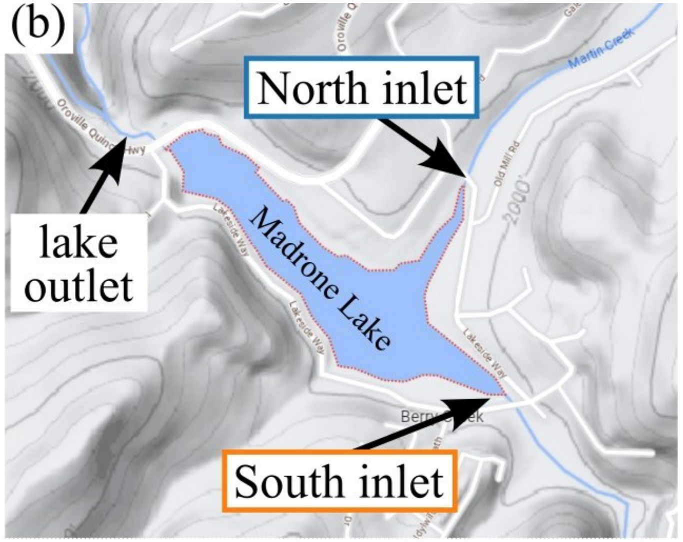
Open-source Design

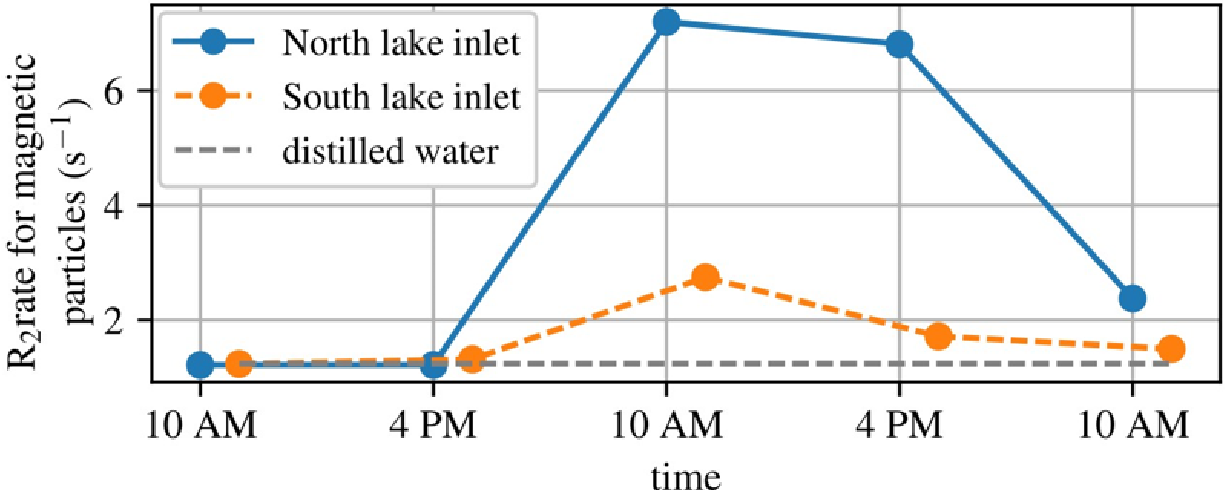
Continuous Water Quality Monitoring

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





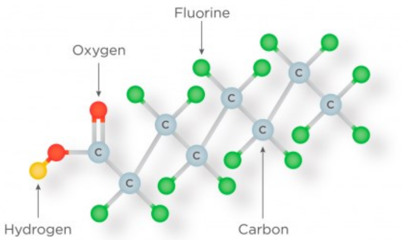


Proposed NMR Use Cases

immediate objective	short-term objective	medium-term objective	long-term objective
continuous Monitoring (heavy metals)	wildfire and coal ash detection	algae blooms	PFAS

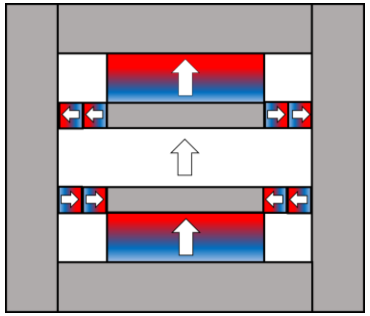




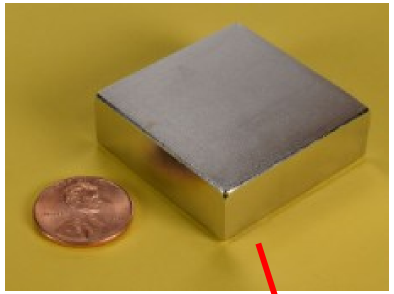


Permanent Magnet Array

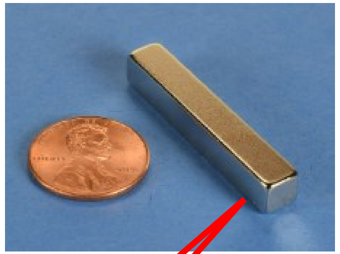
- **0.565 T** strength at 23ºC
  - -800 ppm/K gradient
- Larmor (operating) frequency:
  - $f_{Larmor} = \gamma B = \left(42.58 \frac{MHz}{T}\right)(0.565\ T) \approx \mathbf{24\ MHz}$
- 150 ppm homogeneity
- 4.4 lbs

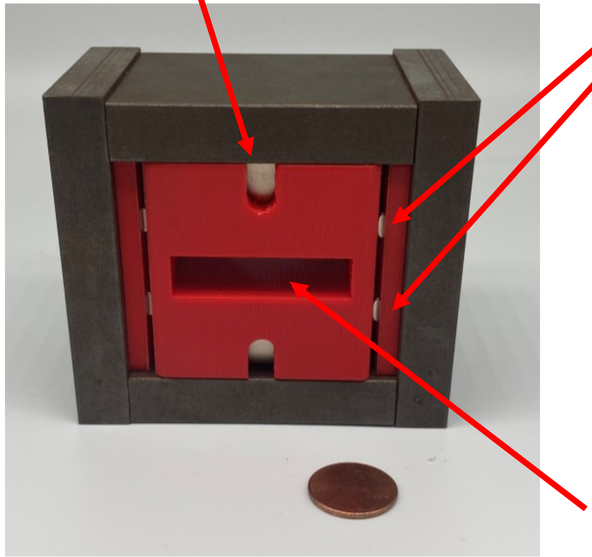


N42 magnet



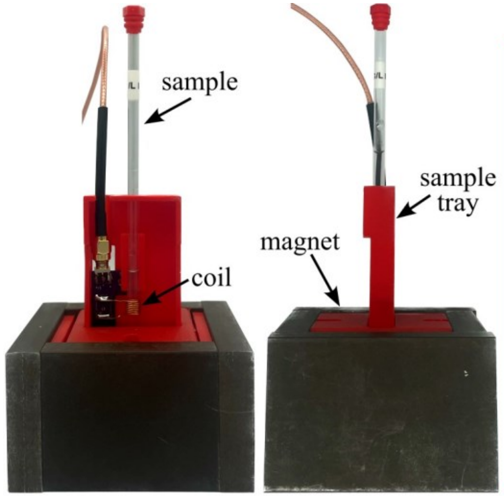
N42 magnet

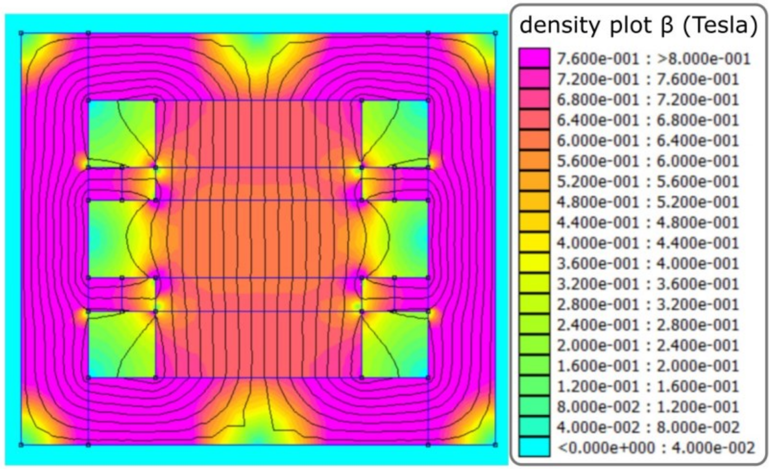




Sample location

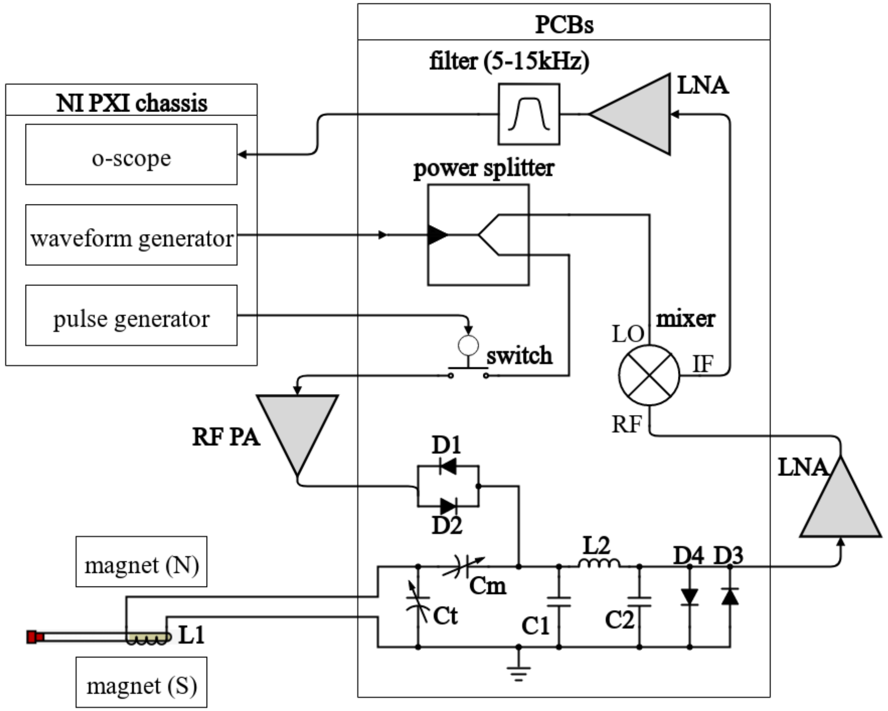
Fully assembled





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

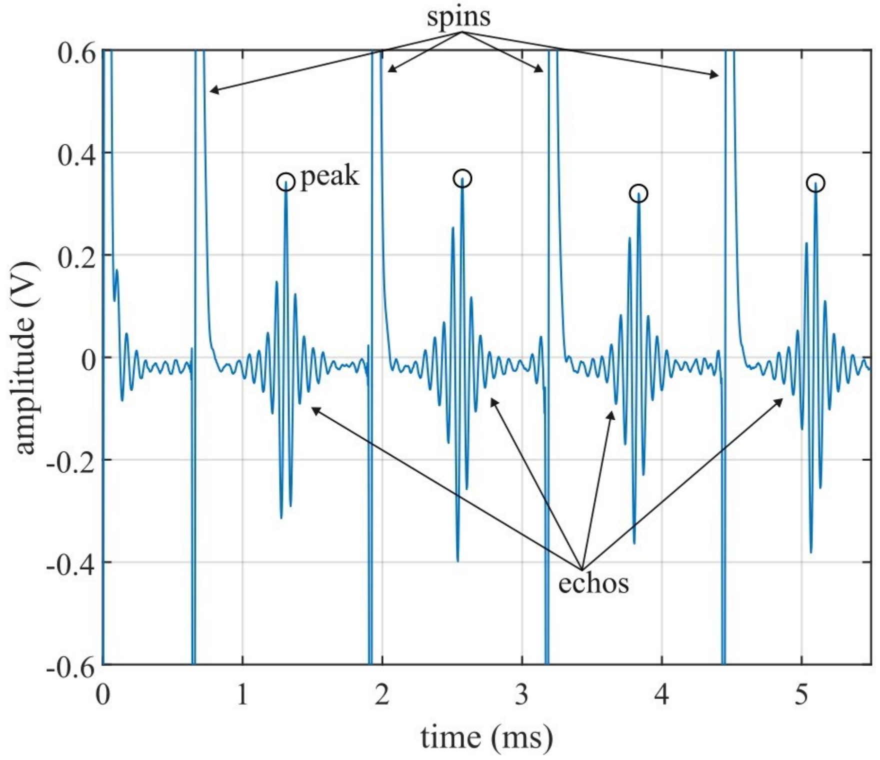


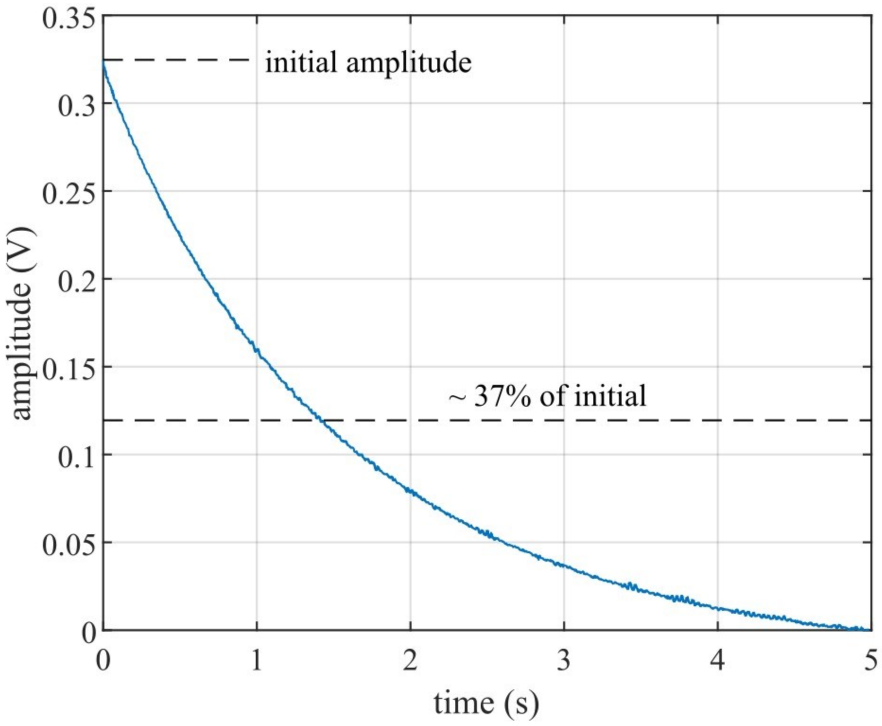
General flow

excitation → NMR response → amplification → mixing → filtering

TD-NMR Signals

- T_2 relaxation modeled as $M_{\text{xy}}(t) = M_0 \exp(-t/T_2)$
- 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

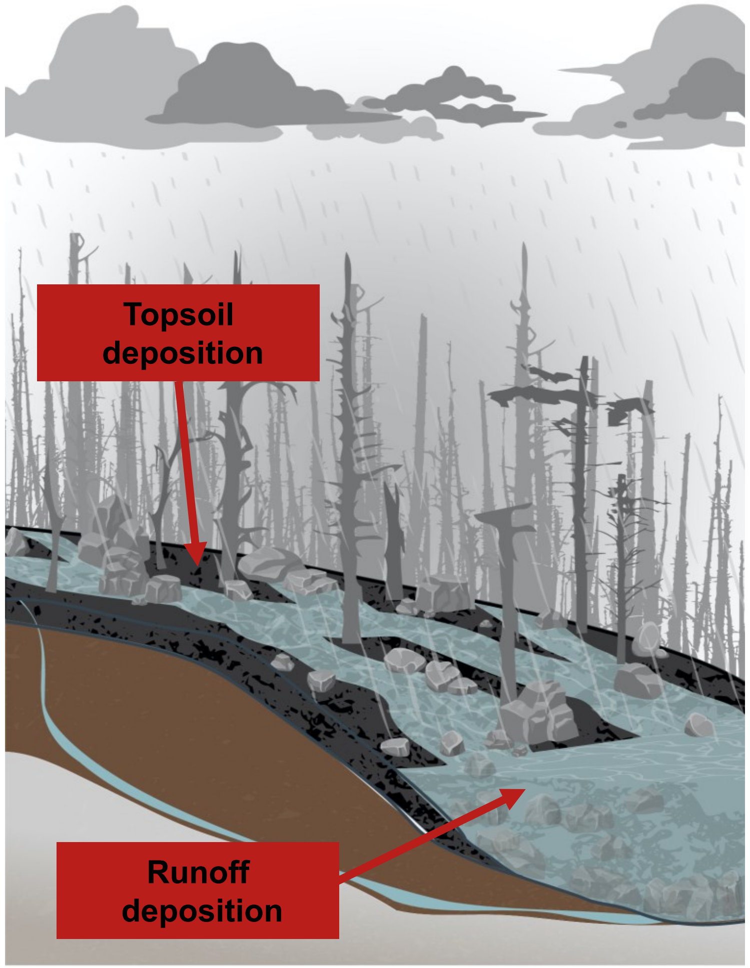




Use Case: Wildfire Ash

Why Monitor Magnetic Contents of Wildfire Ash?

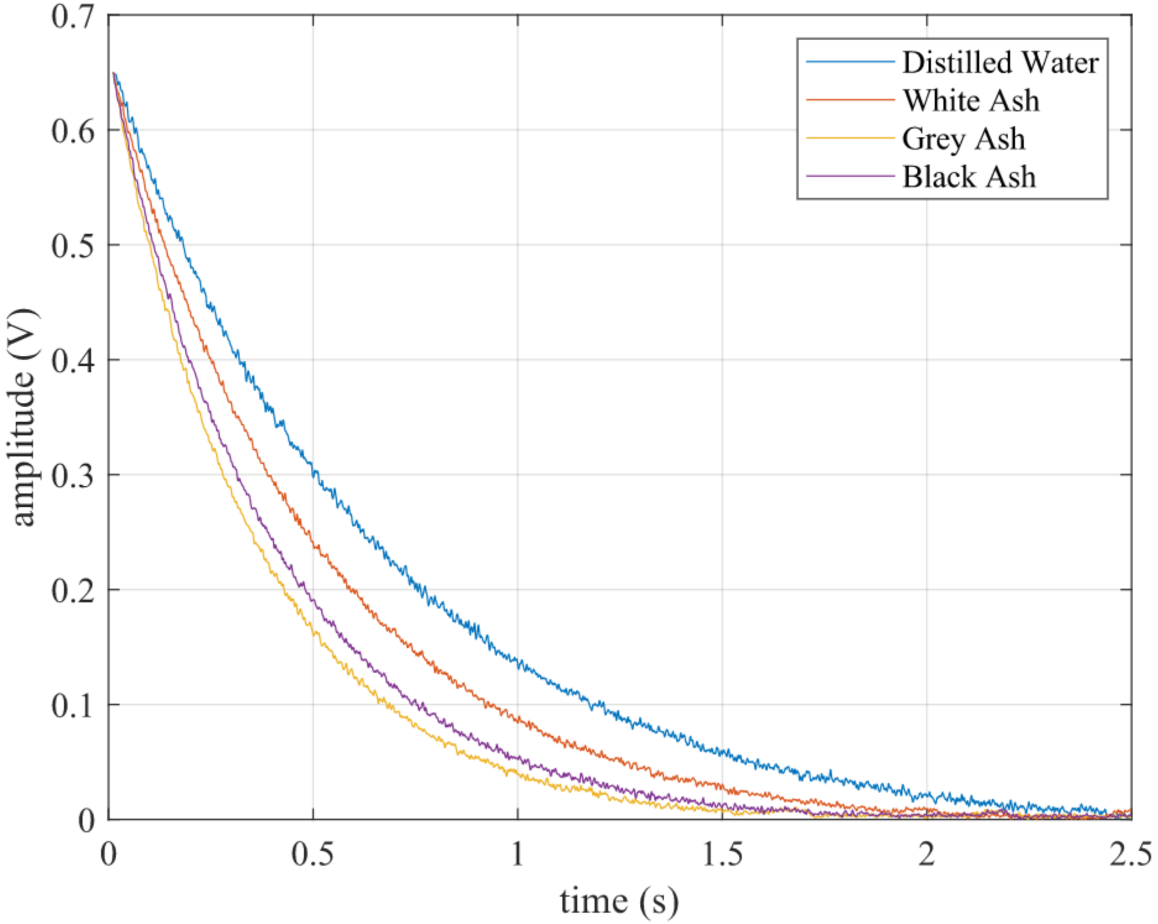
- Effects on topsoil
  - Ash deposits enhance magnetic content in soil
  - Magnetic properties are closely related to climate & rainfall
- Deposition through runoff water
  - Nearby bodies of water accumulate magnetic content
  - Nanoscale magnetite is linked to brain disease
- Understand fire severity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

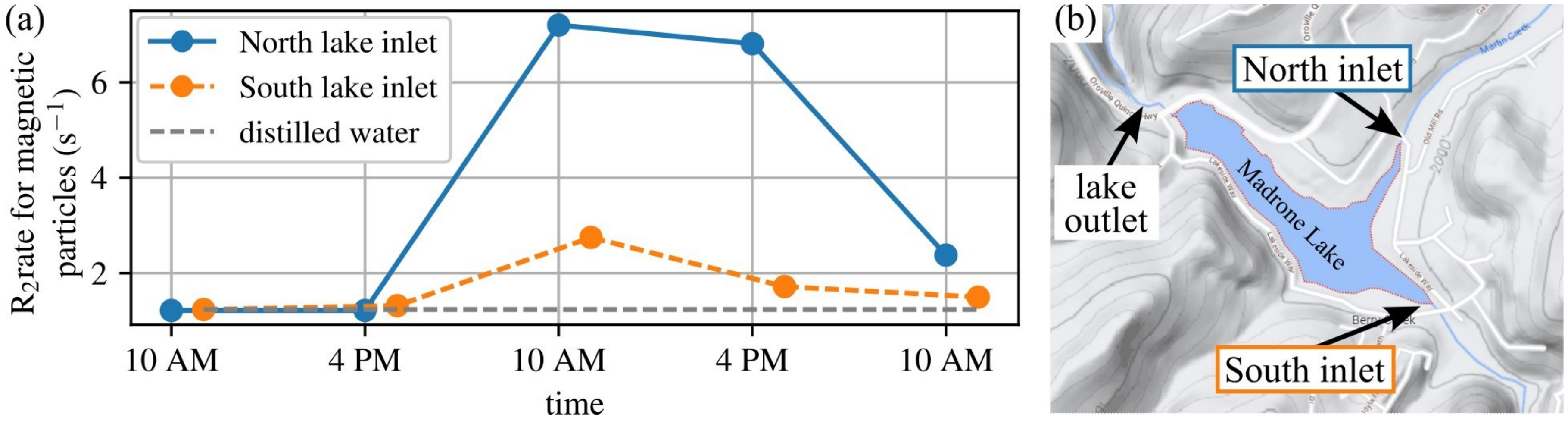
NMR Relaxometry with MPs

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



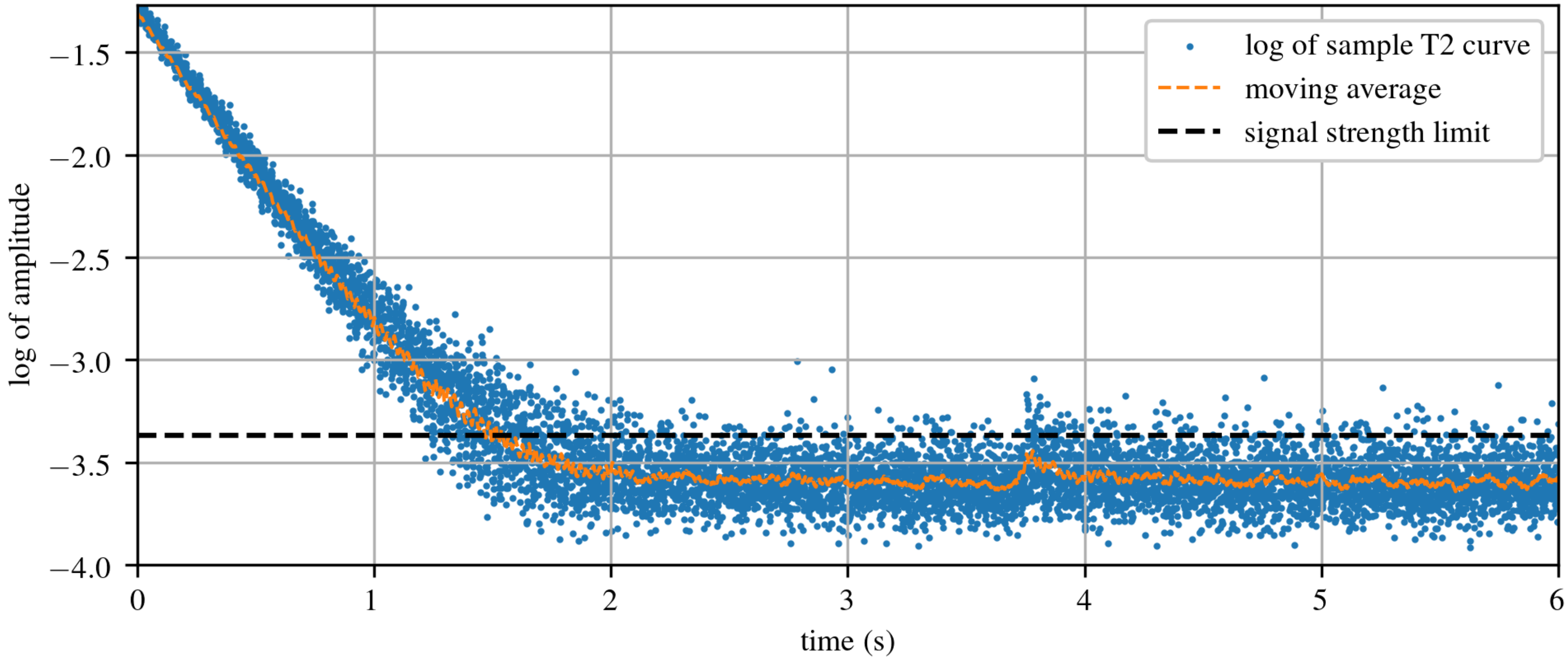
Real-time In Situ Tracking

- 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



Separating Signal from Noise

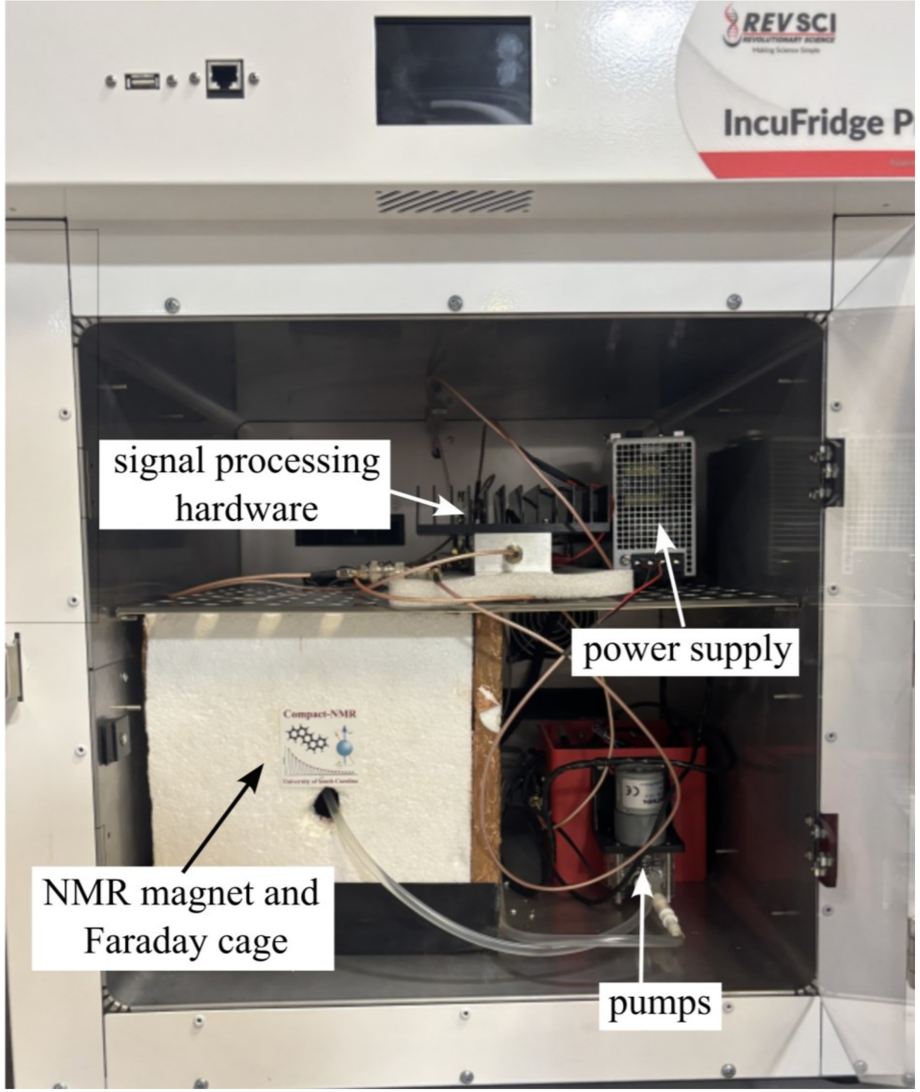
- Natural logarithm of T2 signal allows for the separation of signal and nose



Lab Data Collection for Model Training

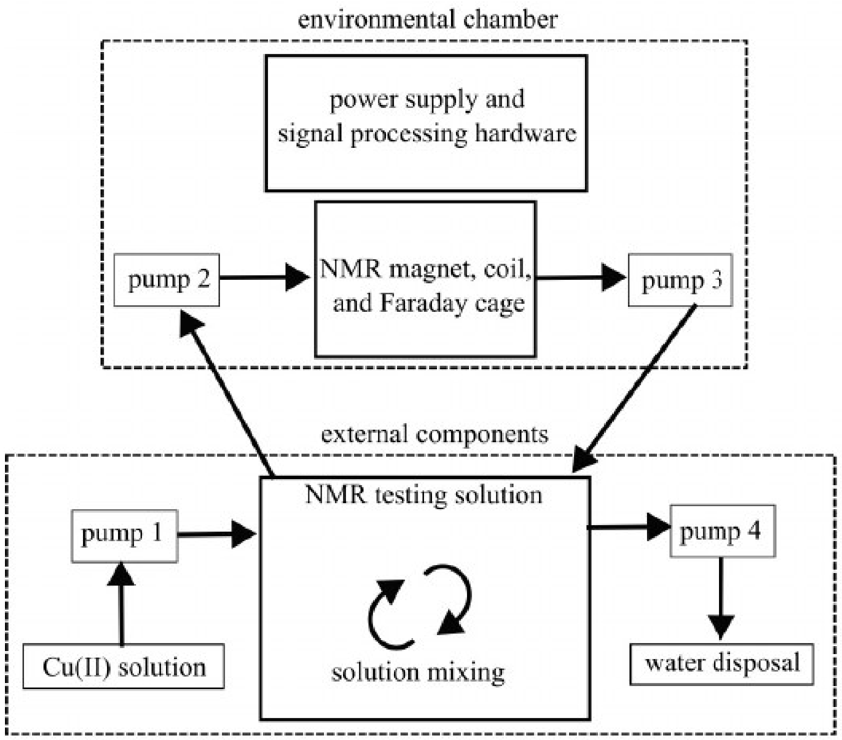
NMR in Environmental Chamber

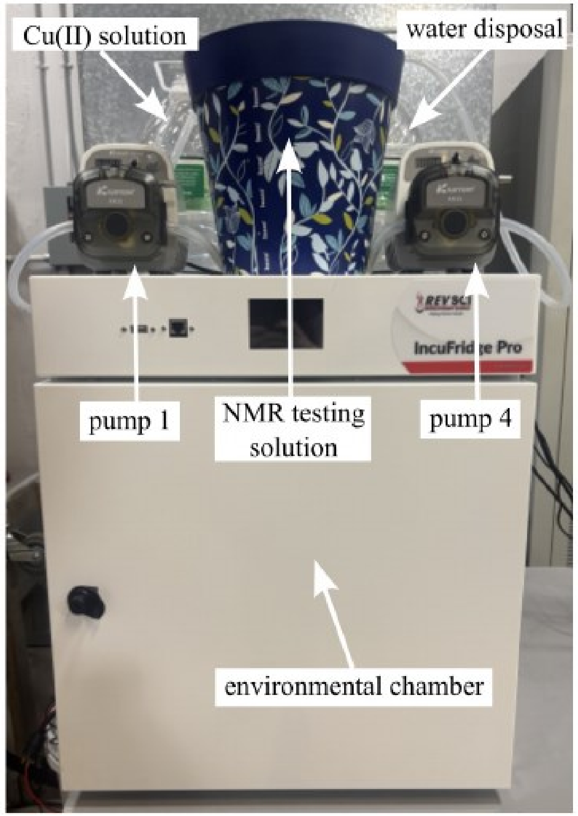
- NMR is placed in an environmental chamber for temperature control.
- Long-term, an environmental chamber would not be easy if the magnet is calibrated over a temperature range.
- Over-sized chamber used for simplicity.



Data Collection for Model Training

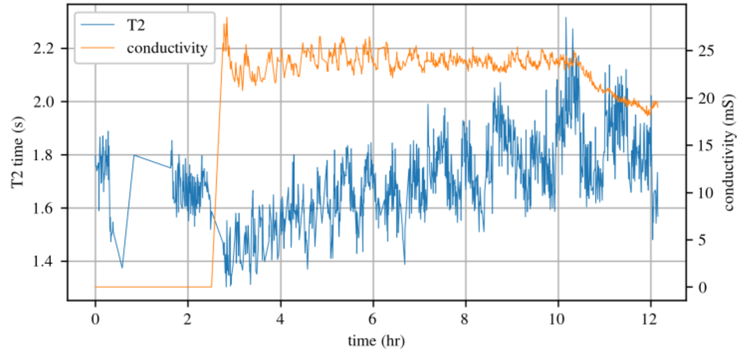
- Data collection method: slowly drip Cu(II) solution into distilled water to provide near-continuous training data
- Remove water at same rate to avoid overflow

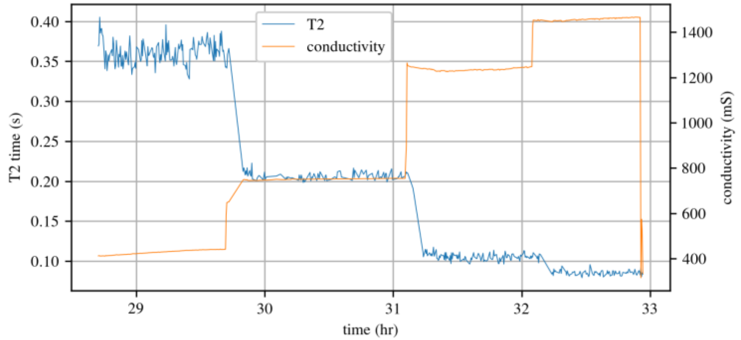


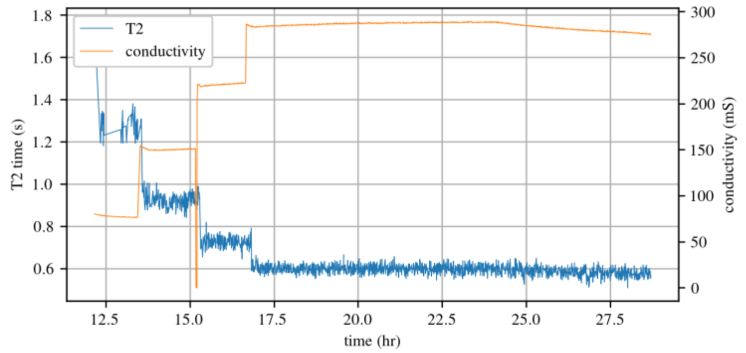


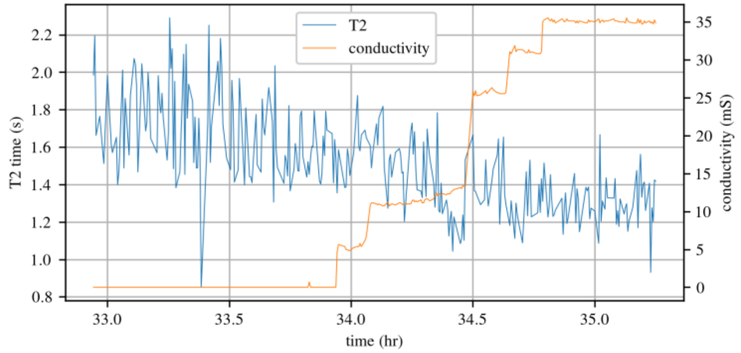
Model Training Data

- Consists of Cu(II) contaminated water from 0mg/L to 1000mg/L
- Stair-step concentration increases to provide model with comprehensive ranges
- Slow and steady increase in Cu(II) contamination at low concentrations to provide near-continuous data





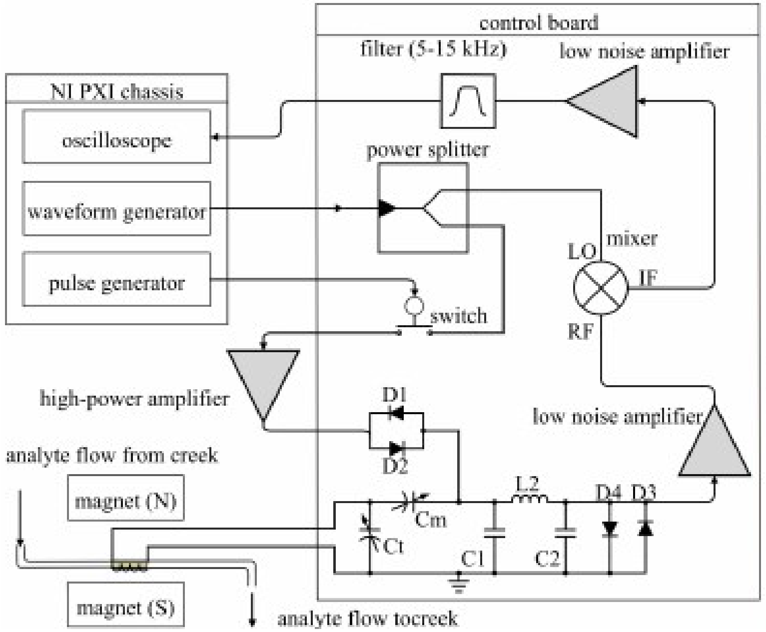


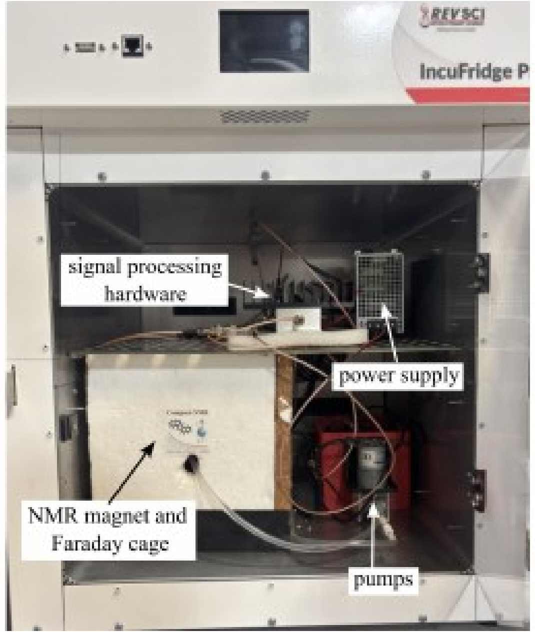


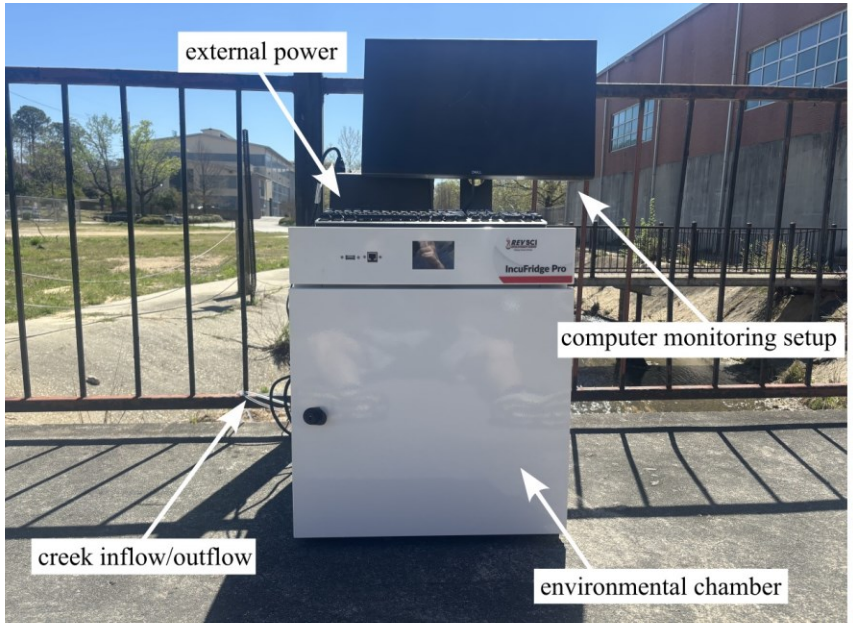
Field Deployment of In Situ NMR system

Field Deployed System

- Environmental chamber: enables temperature control for magnet and RF electronics
- Flow-through pumps: enable automatic sample collection
- NI PXI-8821: enables remote data acquisition with LabVIEW software
- Water quality sensor: measures pH, temperature, turbidity, and conductivity

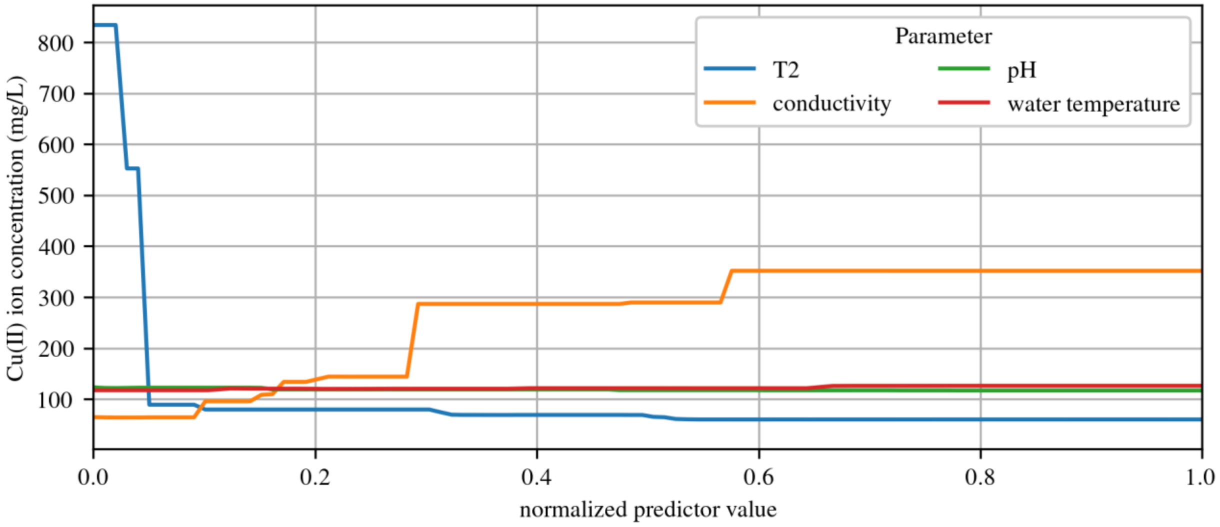


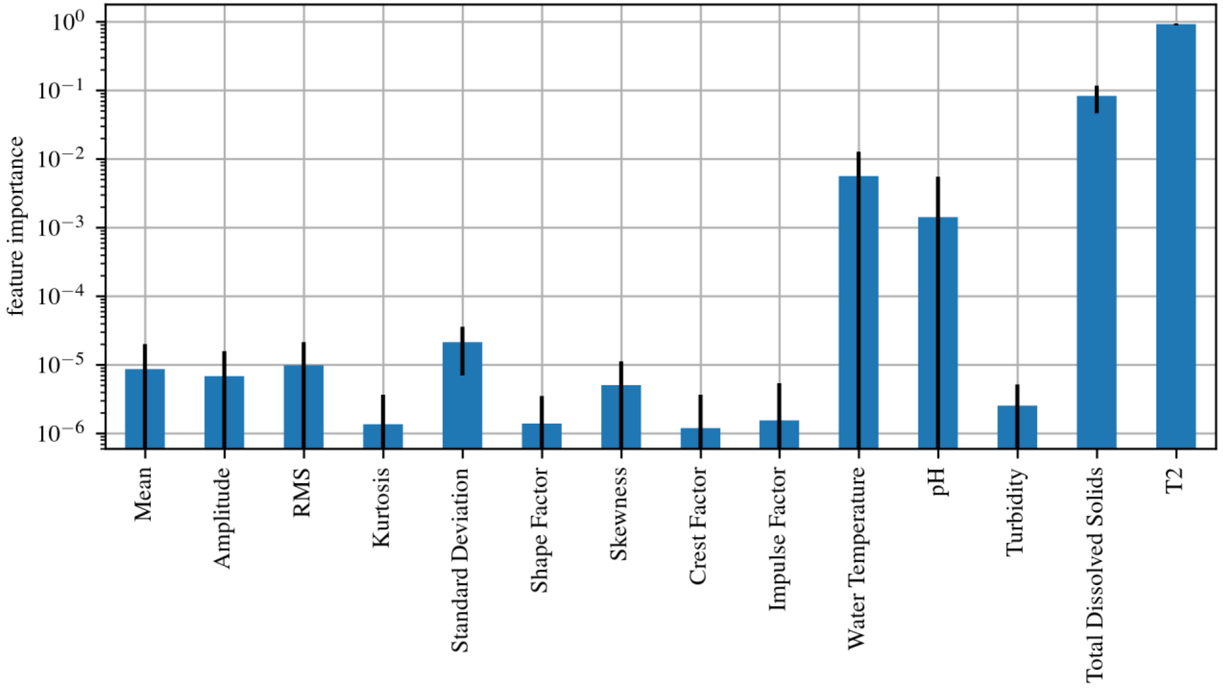




Machine Learning Model

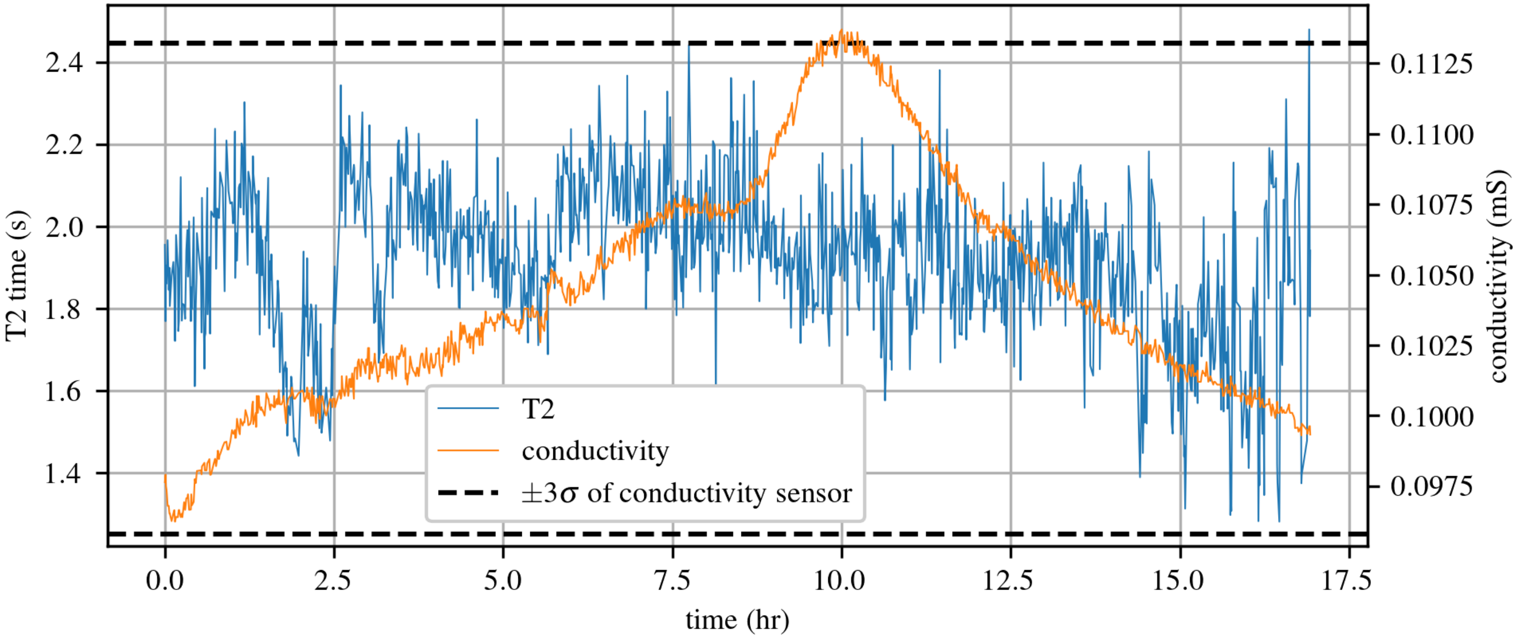
- Partial dependence plot: indicates low T2 and high conductivity cause high Cu(II) concentration and high T2 and low conductivity cause low Cu(II) concentration
- Importance plot: shows that T2 and conductivity are by far the most important
- Together, they indicate the model is thinking correctly

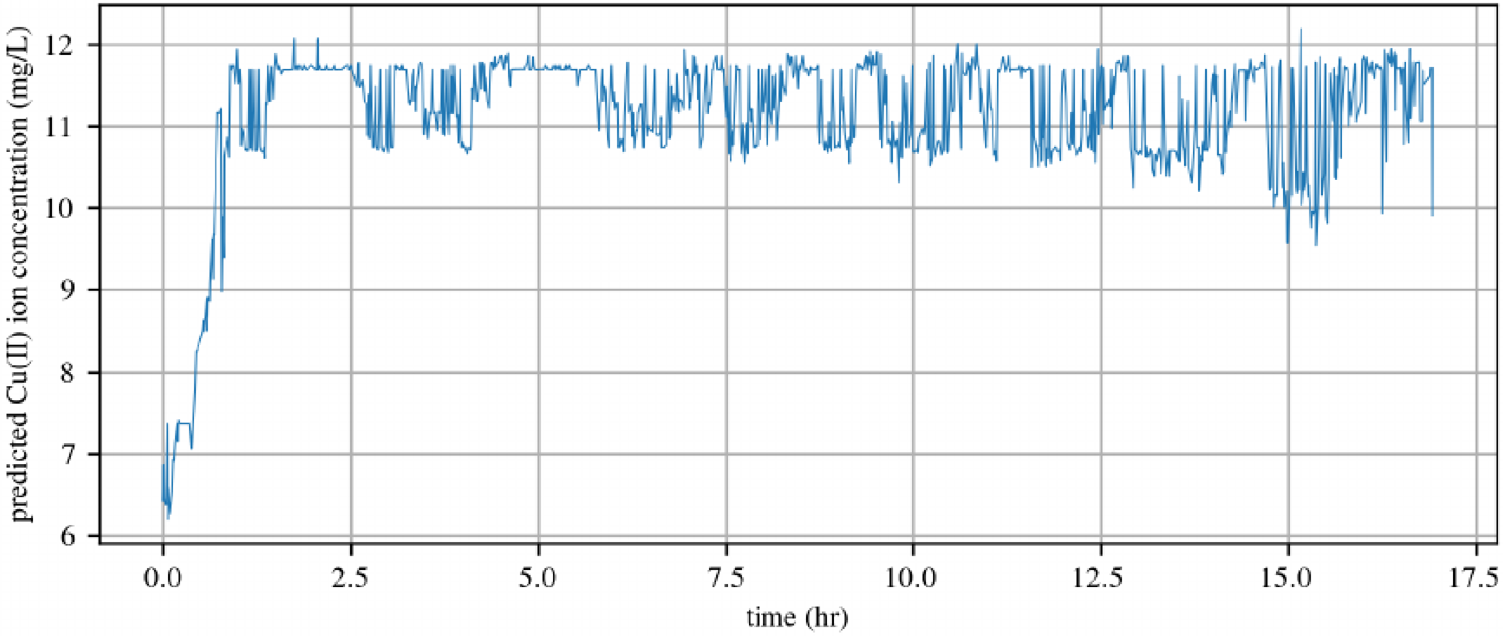




Rocky Branch Creek Data

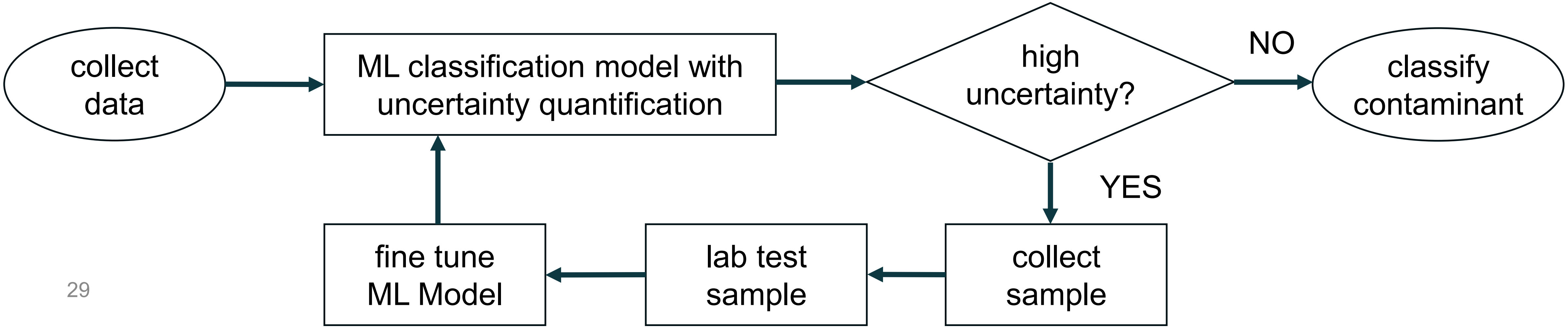
- T2 and conductivity data collected in-situ over 17 hours
- T2 and conductivity (within 3σ) stay the same
- Model predictions agreeing with the consistency of data collection





Future Work: Fine-tuning ML Model

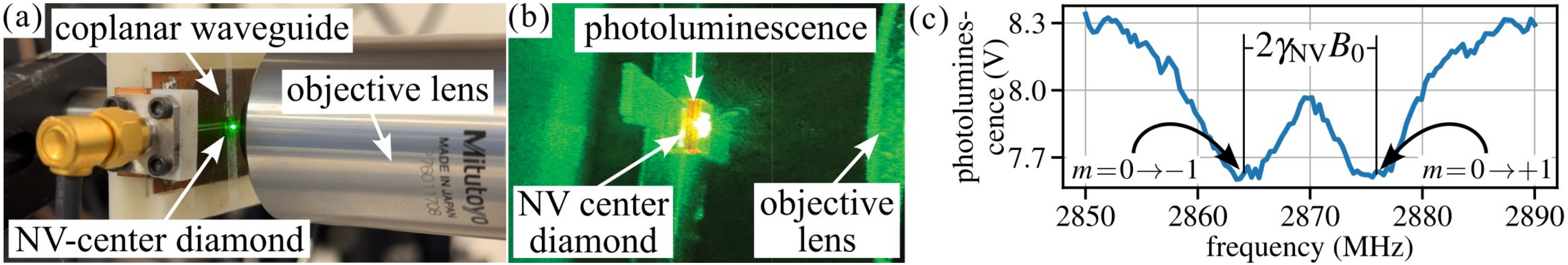
- The flow-through NMR will be deployed with an automatic water sampler and will trigger a sample based on uncertainties in predicted contaminate.
  - Collected samples will be returned to the lab for further assessment.
  - Lab results will be used to fine-tune the model
  - Over time, fewer lab samples 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.



Future Work: Quantum Sensing

We are building a Quantum Sensor (NV center-based) to extend NMR to Optically Detected Magnetic Resonance (ODMR) to enable PPT sensing of PFAS in situ.

- **Operational ODMR on bench:** Confocal microscope + 543 nm pump, CPW microwave drive, and PL readout show clear Zeeman-split dips (Earth-field detection) on a 300 ppb NV diamond chip.
- **Optics/electronics in place:** Green HeNe + AOM, GHz MW source/amplifier, filters/pinholes; PL collected >640 nm with stable counts suitable for control/fit routines.
- **Gaps to close for NMR/ESR:** Need gated timing electronics for laser/MW pulsing and a gated single-photon-level detector



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Thank You for Your Time

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