PhD thesis position

Development of a portable ^{19}F NMR device for the online detection of PFAS in waste water

Supervision:

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Host unit:

- ICube laboratory (EM3 research team) of the University of Strasbourg / CNRS
  https://icube.unistra.fr

Registration: University of Strasbourg (France)

Funding: Wa2MoS ANR/DFG project (April 1st 2026 – March 31st 2029)

Collaborations:

- Institut for Microsystems Technology – University of Applied Furtwangen (Germany)

Starting date: Ideally April 1st 2026, but possibility to start with 6-month Master thesis project before the PhD.

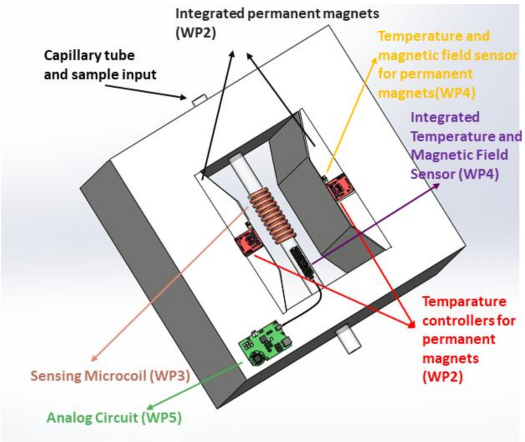
Context: Per- and polyfluoroalkyl substances (PFAS) are synthetic chemicals used since the mid-20th century for their heat, water, and oil resistance [1]. They are found in many products, including cookware, textiles, firefighting foams, packaging, and cosmetics. Their extensive use has caused global contamination of water, soil, and living organisms. Due to their strong carbon–fluorine bonds, PFAS are extremely persistent and are known as “forever chemicals.” Exposure has been linked to serious health issues such as liver damage, fertility problems, immune suppression, hormonal disruption, and cancer. Governments are responding with stricter regulations: France will ban PFAS in certain products by 2026, and Germany advocates tighter industrial controls. These efforts support EU strategies like the Water Framework Directive and the Zero Pollution Action Plan. There is thus a growing need for compact, low-cost, and sensitive PFAS monitoring technologies. The Wa2MoS project aims to address this by combining ICube’s electronic and NMR expertise with HFU’s microsystems know-how to develop a portable NMR-based monitoring solution [2-4]. **More particularly, this PhD project aims at adapting an existing portable NMR system to the detection of PFAS via ^{19}F NMR.**

Project description: NMR measurement consists of acquiring the FID, i.e., the electromagnetic wave resulting from the relaxation of atomic spins which are subjected to a strong static magnetic field $\mathbf{B_0}$, following the application of a transverse radiofrequency (RF) pulse $\mathbf{B_1}$ at the relaxation frequency, i.e., the Larmor frequency. At rest, the spins globally align themselves within the direction of $\mathbf{B_0}$ and precess at the Larmor frequency around the $\mathbf{B_0}$ direction. The RF pulse tilts the sample magnetization which continues to precess around $\mathbf{B_0}$. When the RF pulse stops, the magnetization has been tilted, named the nutation angle which depends on the intensity of $\mathbf{B_1}$ and the duration of the RF pulse. Then, the sample magnetization returns back to its initial position, still through a precession motion. The characteristics of this motion are measured using a coil, most of the time the same as the one used to apply the RF pulse. The resulting signal, so-called FID, contains characteristic frequencies that depend on the minute deviation of $\mathbf{B_0}$ coming from the chemical bonds in the compound. Each chemical compound has thus a specific signature with specific frequencies and intensities. The NMR spectrum, i.e., the Fourier transform of the FID, can thus be analyzed to determine which molecule is in the sample and, eventually, at which concentration.

From a hardware perspective, a NMR spectrometer consists in four main components:

1. a magnet providing the static magnetic field $\mathbf{B_0}$;
2. a coil that enables both the $\mathbf{B_1}$ excitation and the FID measurement ;
3. an electronic circuit for the control, the generation of the RF pulse, and the processing of the FID, and
4. a microfluidic chip to transport and confine the sample in the field of view of the coil and acts as a mechanical support for all the elements integrated in the measurement zone, as described in the sketch on the right.

Each component has a significant impact on the measurement and their contribution to the performances are highly interwoven for instance



- The intensity of the FID increases with the square of $\mathbf{B_0}$;
- The spectral resolution, i.e., the ability to distinguish two close frequencies in the spectrum, decreases with the homogeneity of $\mathbf{B_0}$ (i.e., poor homogeneity corresponds to poor resolution) ;
- The sensitivity S of the detection coil directly affects the intensity of the FID ;
- The field of view of the coil, i.e., the volume V of the sample "reached" by the RF pulse, determines the number of spins that contribute to the signal and thus the amplitude of the FID, but also the volume in which $\mathbf{B_0}$ has to be homogeneous ;
- The accuracy with which the electronics generates the RF pulse (control of pulse duration, inaccuracy in the frequency, jitter) affects the induced precession motion and thus the measured FID upon relaxation.
- The noise of the measurement electronics has a direct impact on the signal-to-noise ratio (SNR) of the FID and therefore on the limit-of-detection (LoD).

Work to be carried out: The project will be structured into four main tasks. The first three tasks can be carried out in parallel.

1. The first task focuses on adapting the existing device for ^{19}F NMR [5-7], including modifications of the probe and excitation/receiving electronics to match the required frequency band and bandwidth. This stage may also involve a redesign of the magnet as well as the design of an ASIC for the analog front-end
2. For optimization purpose and choose the most suitable volume of interest, it is very important to know accurately the 3D map of the $\mathbf{B_0}$ fields in the magnet. For that purpose, we will design an integrated magnetic camera based on 1D Horizontal Hall Devices (HHD) [8].
3. The third task involves using a benchtop NMR to characterize selected PFAS, establishing a baseline, but also develop dedicated signal/data processing algorithm to get retrieve the quantity of interest from the acquired signals.
4. Finally, the fourth task, carried out in close collaboration with HFU, will focus on the integration of all components into a complete and functional sensor.

References :

[1] J. Glüge et al., « An overview of the uses of per- and polyfluoroalkyl substances (PFAS) », Environ. Sci. Process. Impacts, vol. 22, no 12, p. 2345-2373, 2020, doi: 10.1039/D0EM00291G. [Link]

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[3] A. H. Velders et S. Baas, « Shim-free homebuilt 2 T magnet for NMR spectroscopy with sub-ppm resolution and sub-nanomole sensitivity », 2023, Research Square (preprint). doi: 10.21203/rs.3.rs-3303984/v1.

[4] S. S. Zalesskiy, et al., « Miniaturization of NMR Systems: Desktop Spectrometers, Microcoil Spectroscopy, and "NMR on a Chip" for Chemistry, Biochemistry, and Industry », *Chem. Rev.*, vol. 114, 2014, doi: 10.1021/cr400063g.

[5] G. Baumgarten, « Développement et caractérisation d'une sonde RMN portable appliquée au suivi de la qualité de l'eau et à l'étude de la cinétique des réactions chimiques », Thèse de doctorat, Strasbourg, 2024.

[6] D.-V. Nguyen, « Portable nuclear magnetic resonance spectroscopy probe », Thèse de doctorat, Strasbourg, 2020.

[7] L. Werling, « Contribution à l'intégration d'une sonde aiguille haute résolution de spectroscopie localisée par résonance magnétique nucléaire », Thèse de doctorat, Strasbourg, 2022.

[8] Madec, M., Kammerer, J. B., Hébrard, L., & Lallement, C. (2012). An improved compact model for CMOS cross-shaped Hall-effect sensor including offset and temperature effects. Analog Integrated Circuits and Signal Processing, 73(3), 719-730.

Skills required

- Electronics (analog and digital) and microelectronics (ASIC design)
- Signal and data processing
- Computer sciences (C++ for embedded systems, Python)
- Prior experience in instrumentation — particularly in setting up experimental protocols and characterizing instruments — would be an asset.