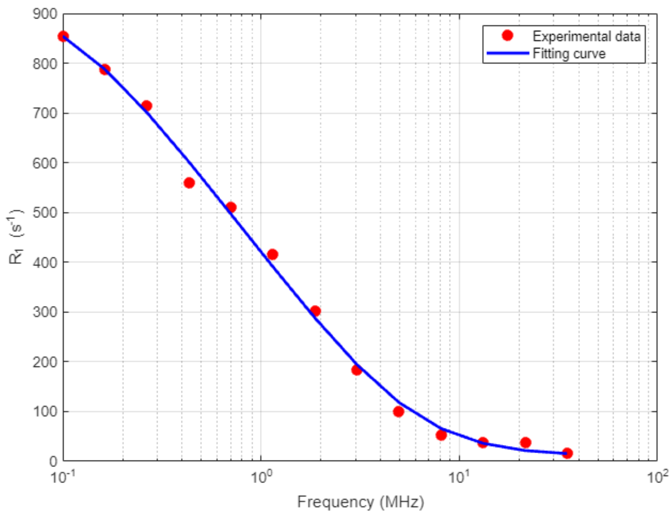
Title: Improvement of tools for interpreting NMRD profiles

Fast Field Cycling-Nuclear Magnetic Resonance (FFC-NMR) relaxometry is a non-destructive low-field magnetic resonance technique which is performed in the range from a few kHz up to around 100 MHz, depending on the instrument. It is the only low-field NMR technique which measures the longitudinal spin relaxation rate, $R_1=1/T_1$ (where T_1 is the NMR longitudinal relaxation time), as a function of the magnetic field strength over a wide range of frequencies using only one instrument[1].

The magnetic field dependence of R_1 is shown graphically as a Nuclear Magnetic Resonance Dispersion (NMRD) profile where R_1 is plotted against the Larmor frequency of the relaxation magnetic field. Below is an example obtained using the homemade software GUI_FFCNMRSolver.



Many materials and environments can be studied with FFC-NMR technique, such as:

- Proteins;
- Monoclonal antibodies;
- Polymers;
- Electrolytes and ionic liquids;
- Liquid crystals;
- Environmental samples;
- Foodstuffs;
- Porous materials;
- Hydration process of cement;
- Diffusion measurements.

Two FFC-NMR instruments are installed at the DICAM’s LAGIRN NMR-laboratory, the newest and upgraded as part of a PNRR project. They are mainly used to study porous media (usually rocks and cementitious materials, but also foodstuffs).

The information obtained from T_1 is related to the molecular dynamics of the measured sample. In particular, the FFC-NMR technique is useful for revealing information on slow molecular dynamics which can only be carried out at very low magnetic field strengths[2].

In principle, the relaxation rate R_1 of a substance will tend to change when there is a variation in molecular dynamics, which may be caused by:

• change of state (e.g. solid to liquid; phase changes in complex systems such as liquid crystals);

• concentration changes (e.g. effect on aggregation states of biomolecules);

• temperature changes;

• viscosity changes;

• cofactor interactions such as sulfur-polymer coupling or plasticizer effects;

• paramagnetic impurities;

However, extracting useful information from the measured samples requires advanced molecular dynamics models to interpret the acquired NMRD profiles and powerful software that allows users to invert the NMRD curves.

Over time, researcher in the DICAM NMR laboratory worked on the development of dedicated FFC-NMR software tools. In particular, two software are now freely available, although still under development: ModelFreeFFC and GUI_FFCNMRSolver [3, 4, 5]. Their use for the study of cement samples is of particular interest[6,7].

Scope of the research

The purpose of the research project is to enhance the inversion of NMRD profiles by improving the pre-processing of raw data, extending the performance of the homemade inversion software tools developed at DICAM (ModelFreeFFC and GUI_FFCNMRSolver), and applying them to the characterization of curing-induced effects on the structure of WPC (White Portland Cement) samples.

Activity plain

All activities will be carried out at the LAGRIN NMR laboratory at DICAM using the Stelar FFC-NMR relaxometer at the DICAM NMR laboratory.

WPC samples preparation, with different w/c ratio, and initial ^{1}H NMR relaxometry characterization during the first month of underwater hardening (1˚ months);

Tuning and calibration of NP and PP FFC-NMR sequences used to acquire the cement FFC-NMRD profiles (1˚ to 3˚ month);

Improvement of the data extraction from raw PP and NP data to create the NMRD profiles (from 3˚ to 9˚ month);

Testing and evaluating of possible improvement of the homemade ModelFreeFFC and GUI_FFCNMRSolver inversion tools used to invert cement NMRD profiles (from 4˚ to 11˚ month);

Preparation of the final report (12˚ month).

References

1. G. Ferrante, S. Sykora. Technical aspects of Fast-Field Cycling, Advances in Inorganic Chemistry, 57, 405-470, 2005;
2. R. Kimmich, E. Anoardo. Field-Cycling NMR Relaxometry, Progress in Nuclear Magnetic Resonance Spectroscopy, 44, 257-320, 2004;
3. F. Zama, G. Landi, G. Vito Spinelli, L. Brizi, C. Testa, A. Nagmutdinova, V. Bortolotti. ModelFreeFFC Tool: inversion method and software for the analysis of NMRD profiles. 12th Conference on Fast Field Cycling NMR Relaxometry, 2022.
4. G. Vito Spinelli, F. Zama; G. Landi; L. Brizi; C. Testa, A. Nagmutdinova, V. Bortolotti. Inversion method for the analysis of NMRD profiles by means of the software tools ModelFreeFFC and MFMUPenFFC. Italian - French International Conference on Magnetic Resonance, jointly organized by GERM and GIDRM, 2022.
5. V. Bortolotti, L. Brizi, A. Nagmutdinova, F. Zama, G. Landi. MUPen2DTool: A new Matlab Tool for 2D Nuclear Magnetic Resonance relaxation data inversion. SoftwareX, Open Access, Volume 20, 2022
6. V. Bortolotti, L. Brizi, R. J. S. Brown, P. Fantazzini, M. Mariani, Nano and Sub-nano Multiscale Porosity Formation and Other Features Revealed by ^{1}H NMR Relaxometry during Cement Hydration. Langmuir 30, 10871−10877, 2014.
7. A. Nagmutdinova, L. Brizi, P. Fantazzini, V. Bortolotti. Investigation of the First Sorption Cycle of White Portland Cement by ^{1}H NMR. Applied Magnetic Resonance, Open Access, 52, 12, 1767 – 1785, 2021.