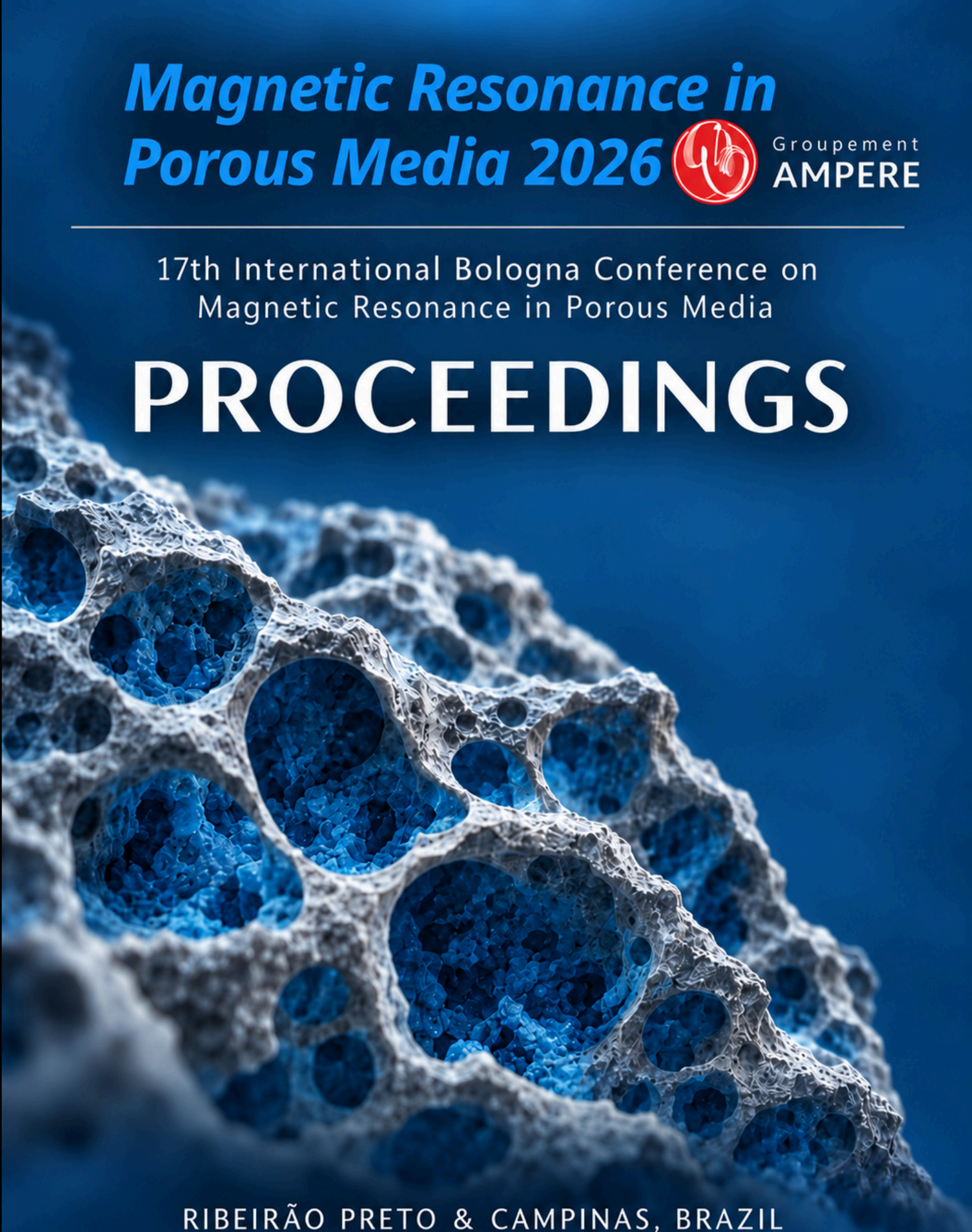
Magnetic Resonance in Porous Media 2026

Groupement AMPERE

17th International Bologna Conference on Magnetic Resonance in Porous Media

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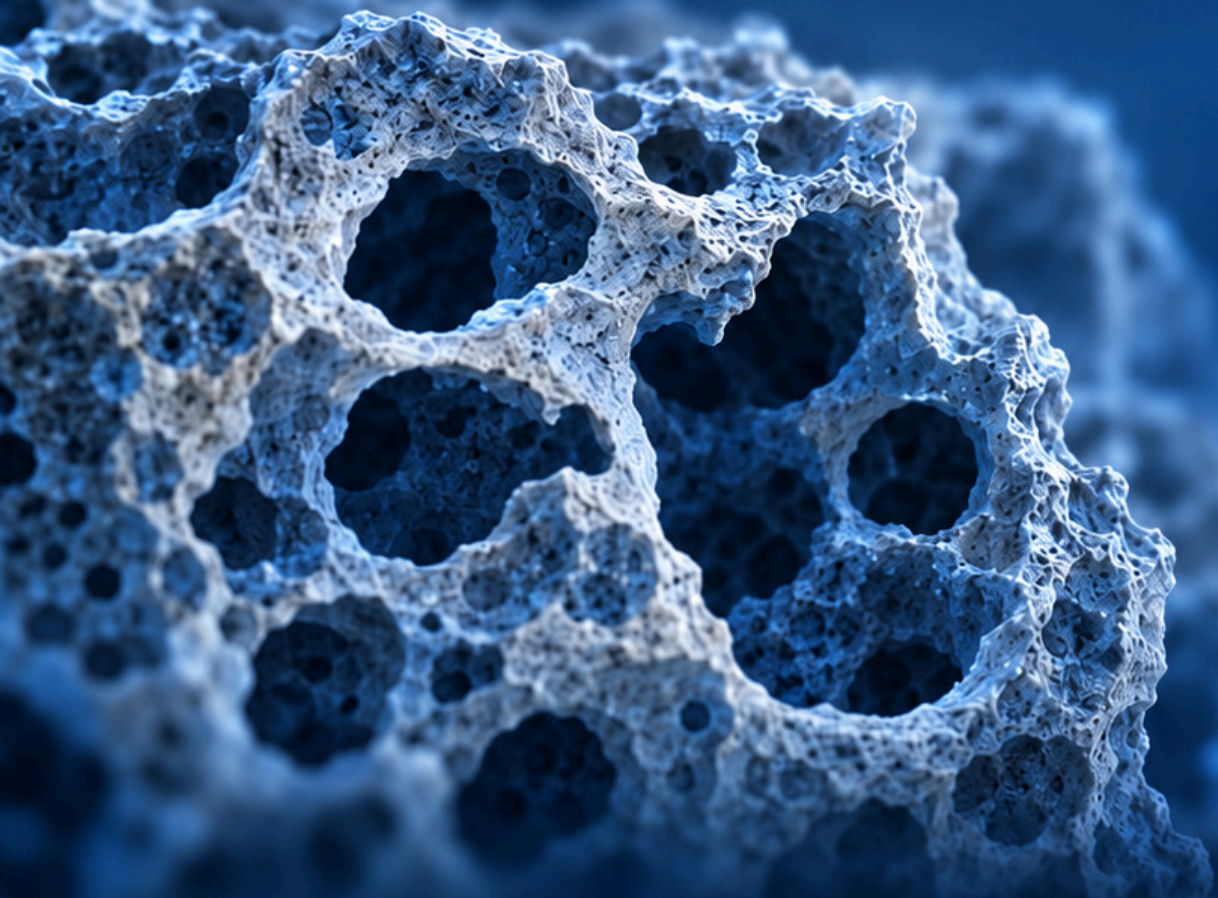
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Digital Porous Media & NMR

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RIBEIRÃO PRETO & CAMPINAS, BRAZIL
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An Overview of SIRIUS, the Brazilian 4th Generation Synchrotron Light Source

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SIRIUS is the synchrotron light source of Centro Nacional de Pesquisa em Energia e Materiais (CNPEM), operated by the Brazilian Synchrotron Light Laboratory (LNLS). It is a 3 GeV diffraction-limited storage ring designed to deliver highly brilliant, stable, and coherent X-ray beams to a diverse suite of beamlines dedicated to imaging, scattering, spectroscopy, and time-resolved experiments. This contribution presents an overview of the facility, its design principles, and its experimental capabilities, highlighting opportunities enabled by multiscale and in situ/operando approaches. Particular attention is given to research on porous and heterogeneous materials, where synchrotron X-ray methods provide strong complementarity to Magnetic Resonance techniques by accessing pore architecture, structural and chemical heterogeneity, interfaces, and their evolution under realistic conditions. Together, these capabilities position SIRIUS as a platform for integrated, cross-scale studies of complex materials and transport processes.

Bridging Digital Porous Media and NMR

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NMR relaxation measurements provide powerful, non-invasive probes of porous media microstructure, yet their interpretation remains challenging due to the complex interplay of surface relaxation, diffusion coupling, internal magnetic field gradients, and heterogeneous relaxation regimes. Traditional interpretation frameworks rely on simplifying assumptions that often break down in realistic reservoir rocks. This presentation demonstrates how integrating high-resolution imaging with physics-based forward modeling enables robust extraction of intrinsic physical properties and advanced interpretation of NMR responses.
A workflow is presented combining micro-CT imaging, random walk simulations, and Bayesian optimization to bridge the gap between digital rock physics and NMR petrophysics. Random walk algorithms on high-resolution segmented images naturally incorporate structural heterogeneity and diffusive motion without limiting assumptions. This enables quantitative assessment of effects like diffusion coupling between different relaxation regimes and the influence of internal gradients at varying field strengths.
Applications are illustrated for Bentheimer sandstone using a Bayesian optimization framework. First, NMR T2 relaxation measurements are matched by simulation and surface relaxivity of quartz and effective relaxation and effective diffusion properties of clay regions are simultaneously extracted. Second, the framework is applied to dual T1 and T2 relaxation measurements extracting 5 parameters and extended to T2 measurements at two different temperatures, extracting surface relaxivities, effective clay relaxation times and effective diffusion coefficients significantly. Finally, I will discuss an analysis of internal gradient effects and microstructure distributions on an artificial “soil” sample at fuall and partial saturation.

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C.H. Arns & I. Shikhov, New Developments in NMR: NMR in Plants and Soils 37, 58-84 in “New Developments in NMR: NMR in Plants and Soils”, Royal Society of Chemistry, 2025

Dual high-field NMR approach to oil-water quantification in porous rocks

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The oil industry plays a pivotal role in identifying promising exploration areas to enhance hydrocarbon recovery and reduce drilling costs. Although much effort has been made to achieve these goals, the success rate still remains significantly below the desired one and, in some cases, a success of 20 % has been reported. In this context, high-field nuclear magnetic resonance imaging has attracted growing interest for being noninvasive, possessing a high signal-to-noise ratio, and enabling oil and water identification in porous rocks [1]. In this work, we produced microporous rocks with grain sizes in the range of 75-125 µm, 150-212 µm , 250-300 µm for oil and water saturation in different fractions. The spectra showed consistently two broad peaks for water (≈ 0.5 kHz) and oil (≈ 1.0 kHz), enabling chemical shift contrast. From this, we could spatially resolve water and oil, obtaining information on fluid conformation. Signal decay experiments were undertaken using the CPMG pulse sequence protocol. We observed that the water signal decays faster than the oil signal, allowing relaxation imaging-based contrast. T2-weighted imaging was employed using the RARE protocol. From the signal segmentation and pixel counting, we could quantify oil and water fractions across 100 rock samples for comparison with known fluid saturation volumes. Our protocol allowed an error of less than 12 % for all samples. These findings suggest that magnetic resonance imaging can serve as a complementary logging tool for well analysis.

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This study was financed by Petrobras

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Dual-Scale Simulation of NMR Responses in Chalk

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Dual-Scale Simulation of NMR Responses in Chalk

Chalk formations constitute important targets for CO2 geological storage in depleted oil fields, yet their complex pore networks spanning nanometer to micron scales pose significant challenges for NMR characterization. Understanding how internal magnetic field gradients and multi-scale porosity heterogeneity influence relaxation responses is essential for reliable interpretation of NMR measurements in these formations. This presentation details a sophisticated dual-scale numerical simulation approach designed to capture these effects in chalk microstructure.

The simulation methodology combines micro-CT imaging at 3.62 µm resolution with Gaussian Random Field (GRF) reconstruction of nano-CT data at 64 nm resolution. The micro-CT image is segmented into three phases: resolved macroporosity (vugs), intermediate unresolved porosity, and semi-solid inclusions. The GRF approach enables periodic generation of the fine-scale microporosity, matched to experimental nano-CT images through two-point correlation functions. This dual-scale representation is utilized by a random walk algorithm where the microstructure is generated on-the-fly rather than storing the complete high-resolution volume. The internal fields are computed using dual-scale FFT methods, capturing both fine-scale heterogeneity within microporosity and long-range gradients from larger-scale susceptibility variations.

Results demonstrate significant effects of paramagnetic inclusions on T_2 relaxation distributions. Even at low field strength (2 MHz), moderate inclusion fractions with susceptibility contrasts of up to 0.01 SI produce significant distribution shape changes. CPMG simulations at multiple echo spacings (0.1-1.0 ms) reveal the echo-spacing dependence of gradient refocusing, distinguishing fine-scale from large-scale internal field effects, and enabling quantitative assessment of their relative contributions to observed relaxation behaviour.

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Estimating surface relaxivity as a function of pore size via conditional diffusion models

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Pore size distribution is a fundamental deliverable of Nuclear Magnetic Resonance (NMR) for reservoir rock characterization. Typically, it is determined in the fast diffusion regime via the surface-to-volume ratio and surface relaxivity (ρ). Although conventional methods rely on a uniform relaxivity assumption, it is highly unlikely that heterogeneous sedimentary rocks exhibit uniform mineralogy across all pore surfaces (Keating and Knight, 2012). To investigate how ρ varies as a function of pore size, we adopt an inverse problem framework (Benavides et al., 2017) to recover the relaxivity function whose corresponding simulated T2 distribution best matches the ground truth T2 distribution. Because standard iterative inversion frameworks require computing forward NMR simulations at each step, they may be computationally prohibitive. To overcome this limitation, we employ generative conditional diffusion models to solve the inverse problem using a data-driven approach. The model takes a rock sample's microstructure image and its experimental T2 distribution as inputs to predict the underlying relaxivity function. To build a robust training dataset, we adopted a sigmoid prior assumption for the relaxivity functions and utilized an in-house Random Walk (RW) simulator to generate the transversal NMR relaxation signals. Importantly, since the total number of wall collisions of a walker in an RW simulation correlates with the local pore size, we parameterize ρ as a function of the collision count rather than mapping it directly to complex pore coordinates. Tested on synthetic data, the proposed framework successfully reconstructed the non-uniform relaxivity functions, providing a significantly better match to the reference T2 distributions than the uniform relaxivity assumption and demonstrating high potential for accurate porous media characterization.

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Magnetic resonance imaging of acid-induced wormholes in carbonate rock: three-dimensional morphology and its control on flow capacity

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Matrix acidizing creates dissolution channels (wormholes) whose 3D morphology sets the conductivity a treatment delivers, yet it is usually inferred from breakthrough data rather than measured. We imaged six acidized Indiana limestone plugs by magnetic resonance and used the geometries directly as the computational domain for flow simulation. The plugs came from corefloods at 0.5-5 mL/min with nonionic acid nanoemulsions carrying 15 wt.% HCl. After saturation with deionized water, volumes were acquired at 2 T (Bruker Avance III) with a T2-weighted 3D gradient-echo sequence tuned to water in large voids: TE 15 ms, TR 30 ms, flip 60 deg, FOV 96x48x48 mm3, 200 um isotropic, 16 averages, 8 h per plug. Since the signal comes from the saturating fluid, the channel is recovered without contrast agents or a reference scan. A new processing step separates it from the free-water films coating the plug, which hold an order of magnitude more volume. Channels are labelled W1-W6 by decreasing median local thickness (2.38-0.74 mm; tortuosity 1.52-2.23). Three patterns emerge: a wide, sparsely branched dominant channel (W1, W3); a ramified dominant channel with bifurcations, loops and enlarged dissolution regions (W2, W4, W5); and a distributed network (W6) reaching the outlet through three mouths carrying 35/35/30% of the flow. The geometries were meshed and solved with the steady Navier-Stokes equations at ten rates, 0.1-200 mL/min, in both directions (120 simulations). Permeability scales as d50^1.94, recovering the Poiseuille exponent from the images, and one tortuosity correction predicts it to 15%. Between 13 and 34% of the dissolved volume carries no flow, and the pressure drop is up to 67% higher against the direction of treatment. MRI therefore distinguishes wormhole morphologies while showing only the water-accessible network, and supplies a geometry from which treatment conductivity can be computed.

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MOGNO Beamline and Applications in Porous Materials

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The MOGNO beamline at the SIRIUS synchrotron is designed to enable fast, high-resolution 3D and 4D imaging using multiscale X-ray micro- and nanotomography. Its optical layout and flexible operation modes allow users to probe materials across a wide range of length scales, combining submicrometric spatial resolution with large fields of view and enabling fast acquisition for time-resolved 4D imaging.
Porous materials benefit significantly from these capabilities, as their performance often depends on complex, multiscale pore networks. MOGNO enables detailed characterization of pore morphology, connectivity, and transport-relevant features across micro- and nanometric domains. Applications include studies in catalysis, energy materials, geology, construction materials, and filtration media. By integrating advanced imaging modalities with robust reconstruction and analysis tools, MOGNO provides a powerful platform for unveiling structure–property relationships in porous systems.

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NMR and Digital Porous Media in the MOGNO beamline

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The fourth-generation Brazilian Synchrotron Light Laboratory (LNLS/Sirius, CNPEM, Brazil) delivers low- to high-energy X-rays with high photon flux, enabling fast high-resolution 3D tomography. The MOGNO beamline [1] at the Sirius/LNLS provides nano- to micrometer-scale computed tomography, including multiscale and zoom tomography with ~200 nm resolution, as well as 4D in situ imaging with time resolution of a few seconds. Designed for flexible sample environments, MOGNO operates at 22, 39, and 67 keV and supports research in materials and energy sciences, including studies of rocks and porous media relevant to the oil industry and CO_2 storage. Current efforts focus on integrating micro-tomography with complementary techniques to investigate pore-scale transport and fluid–surface interactions. Nuclear Magnetic Resonance (NMR) provides fluid characterization and morphological information such as pore-size distribution, connectivity, wettability, and magnetic surface relaxivity [2]. Integrating zoom tomography with NMR offers an important approach to study porous media under static and dynamic conditions. In this talk, we discuss synchrotron-based simulations of NMR signals and the development of an NMR system, in partnership with FIT (Fine Instrument Technology - Brazil) [3], for in situ experiments at the MOGNO beamline.

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Origin and key figures behind Bologna MRPM conference

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The Bologna MRPM conferences grew out of the vision of G.C. Borgia and P. Fantazzini, who in the mid-1980s realized that both petroleum reservoirs and biological materials could be treated as porous media and studied using NMR[1]. Building on the early foundational work in the field, they launched a research program in Magnetic Resonance in Porous Media and organized the first MRPM meeting at the University of Bologna in 1990, at a time when only a few groups worldwide were active in this area. The success of that meeting led to the establishment of a distinguished biennial international conference series, which expanded steadily over the years and eventually became part of Groupement Ampère. In recognition of Bologna's central role, the series was formally named the Bologna Conference, and the Giulio Cesare Borgia Award was created to honor his scientific legacy and encourage young researchers. The MRPM community has grown over the years thanks to the active participation of distinguished members from all over the world, who have demonstrated significant scientific activity. Their names can be found in the contributions to the MRPM Proceedings and as members of the organizing and scientific committees. From the long list, it is both a duty and a pleasure to recognize and honor the two great personalities that have passed away, R.J.S. Brown(1924-2019) and Sir P. T. Callaghan(1947-2012), who made great contributions to both the MRPM conferences and developments of MRPM science and applications. In Bologna, the seminal ideas of the founders have grown and continue to flourish in basic research[2]. The most recent achievements regard the development of one- and two-dimensional inversion methods, FFC data analysis, and AI design for MR Fingerprinting, without neglecting applied research covering a wide range of natural and artificial porous materials (biological tissues, corals, rocks, ceramics, cements, etc.) inside homogeneous and inhomogeneous polarizing magnetic fields.

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Physics-Based Multiscale Modeling of Coal Swelling from NMR Cryoporometry to Reservoir Injectivity

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Unlike saline aquifers and depleted reservoirs, where CO_2 storage relies primarily on structural and residual trapping within a largely passive rock matrix, coal seams store CO_2 through direct adsorption onto the coal matrix itself, coupling storage capacity directly to the swelling-induced permeability decline. Such as role makes coal seams a mechanistically distinct and comparatively CCS target relative to conventional geological formations.
Accurate characterization of coal pore structure is essential for predicting CO_2 adsorption, transport, swelling, and injectivity loss during carbon capture and storage. NMR cryoporometry and (T_2) relaxometry are used to determine pore-size distributions and surface relaxivity across micro- and mesopore scales. These experimental data are combined with density functional theory calculations to quantify fluid–solid interactions, adsorption-induced stresses, and coal-matrix swelling. The resulting nanoscale constitutive relations are incorporated into a multiscale homogenization framework to derive effective poromechanical and transport properties at the reservoir scale. The integrated model links pore-scale adsorption and solvation forces to cleat closure, permeability reduction, and the progressive decline of CO_2 well injectivity.

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Study of the effect of porosity on transport properties in carbonate reservoirs using the Lattice Boltzmann Method

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This work investigates porous media using Digital Rock Physics, a key approach for understanding pore-scale transport in carbonate reservoirs [1]. The objective is to characterize and simulate flow in a digital calcite sample (DRP-252) through a multiscale workflow combining image segmentation (Otsu's method) and Lattice Boltzmann Method (LBM) simulations. The pore geometry was reconstructed from the digital rock image, while the physical properties of the water–decane–butyric acid/calcite system (interfacial tension, density, and viscosity) were obtained from experimental and molecular dynamics data reported in the literature. These properties were mapped into consistent dimensionless LBM parameters and implemented with the explicit-force scheme in the TAXILA-LBM framework [2]. Simulations quantified the influence of pore morphology on flow behavior. An inverse relationship was observed between porosity and tortuosity, with increasing porosity promoting less restrictive flow paths. Absolute permeability showed a nonlinear dependence on porosity, increasing markedly as pore connectivity improved and wall effects decreased. Conversely, low-porosity structures exhibited a sharp permeability reduction due to the closure of critical pore throats, leading to higher tortuosity. Oil recovery efficiency also increased with porosity because more connected pore networks enabled a more uniform displacement process. The extraction rate proved highly sensitive to small porosity variations, demonstrating that subtle structural changes significantly affect recoverable oil volume. Overall, the proposed multiscale framework quantitatively links pore structure to transport properties, showing how porosity governs tortuosity, permeability, and hydrocarbon recovery efficiency in carbonate porous media.

Acknowledgements
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Towards a connection between geometry, phase transition and relaxation in mesoporous materials

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Accurately capturing the full complexity of porous structures, including their topology and structural disorder, remains a central challenge in the study of mesoporous materials. Addressing this challenge requires the use of advanced theoretical approaches that explicitly account for pore-network effects and cooperative phenomena. In this work, we demonstrate how structural information can be extracted from phase transitions occurring within porous materials, including adsorption–desorption and melting–freezing transitions, and identify the key structural parameters governing the shape of the resulting hysteresis loops. We show how pore geometry and spatial correlations between pores affect adsorption and desorption behavior. Furthermore, by analyzing these phase transitions, we predict the transport properties of molecules confined within the material. Finally, we establish a link between melting–freezing behavior and relaxation dynamics in porous structures, demonstrating that relaxation phenomena provide additional opportunities for a more detailed and comprehensive characterization of the internal architecture of porous materials.

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Using Approximate Bayesian Computation (ABC) to analyze uncertainties in relaxometry experiments and their consequences in permeability estimation.

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Nuclear Magnetic Resonance (NMR) techniques enable fast and non-destructive characterization of porous media, ideal for laboratory analysis and well logging in the field. Relaxometry is a technique that stands out among the various NMR tools, as it provides accurate measurements of the medium's porosity, as well as an estimation of pore size distributions within it. However, these observations are subject to noise levels and uncertainties inherent to the process. We propose a combination of Approximate Bayesian Computation (ABC) with reduced-order T2 distribution models as a framework for statistical analysis and uncertainty propagation. The T2 time distribution is decomposed as families of gaussian pore size distributions with uncertainty bounds associated with their medium pore size, standard deviation, and relative contribution for the relaxometry experiment. We show that these uncertainties can be propagated using traditional petrophysical correlations, such as the Kenyon model, thus providing upper and lower bounds to permeability estimations.

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Magnetic Resonance in Porous Media 2026

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SECTION

02

NMR Methods & Instrumentation

ORAL PRESENTATIONS



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CO_2-hydrate formation and dissociation study using an innovative NMR probe at low field.

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In the context of CO_2 storage, injectivity is a critical factor and CO_2 hydrate formation in the near-wellbore region can alter petrophysical properties and hinder gas flow. Understanding the mechanisms governing hydrate formation, whether associated with salt precipitation or not, is essential for predicting its impact and defining optimal conditions to prevent its occurrence. This study investigates hydrate formation and dissociation in porous media using Nuclear Magnetic Resonance (NMR) techniques.

Experiments were conducted using an in-house high-pressure Peltier NMR probe, which provides a pressure range of up to 70 bar. The temperature is controlled via a Peltier system, providing temperature control with a precision of about 0.05 °C. This system can achieve a temperature difference of about 30°C below the reference temperature of the cooling bath. Additionally, it allows for slow temperature ramps (as low as 0.1°C/h), which are essential for observing quasi-static hydrate dissociation at constant pressure and for determining thermodynamic equilibrium points (Teq and Peq). The experiments were conducted on small cylindrical samples (5 mm in diameter, up to 20 mm in length), using model porous media as well as various sandstones and carbonates. A typical output of the experiment is the liquid fraction as measured by NMR vs. temperature.

It is well known that hydrate formation can be detected easily in NMR experiments since the T_2 relaxation time becomes very short. Here we focus on the T_1 relaxation to try to distinguish ice from hydrates; with an apropriate NMR instrument, we show that this is possible since hydrate and ice structures have different T_1 relaxation times around 1s. We also studied the kinetics of hydrate formation and dissociation using step temperature variations. Contrary to expectations, the gas water surface area obtained at different water saturations does not influence the kinetics.

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Development of a benchtop high-resolution Magic Angle Spinning NMR

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Over the last fifteen years we have witnessed a dramatic increase in low-field benchtop NMR applications many of which benefited from high spectral resolution. Nowadays, commercial instruments exist offering linewidths better than 0.5Hz on 5mm tube isotropic liquid samples for a variety of Larmor frequencies up to 90 MHz. The compromise to achieve strong field from permanent magnets is reduced free bore diameter. Although recent work to implement magic angle sample spinning have been reported [1, 2], they focused on reducing the anisotropic broadening from dipolar couplings where modest resolution is sufficient.

Here, we present results obtained with a benchtop high-resolution NMR magnet (0.9T) originally built 2010, having a clear bore of 54 mm, which is integrated with standard shim coils and SB liquids and solid-state MAS probes from superconducting NMR magnets. We demonstrate sub ppm high-resolution operation under fast and slow MAS conditions and showcase the potential of this low-cost technology towards democratizing Magic Angle sample Spinning in applications with minimal sample preparation: metabolomics, materials and food science.

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Development of NMR methodologies for the characterization of source rocks from unconventional oil and gas reservoirs. Applications in the Vaca Muerta formation.

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One of the most relevant energy vectors in Argentina's development and economy is the exploitation of hydrocarbons from unconventional reservoirs, such as those found in the Neuquén Basin, particularly Vaca Muerta. Conventional reservoirs are composed mainly of compacted sandstones with high porosity and permeability, whereas shale-type rocks exhibit very low connectivity, requiring hydraulic fracturing for their exploitation. A second major difference is the large amount of solid organic matter present in these reservoirs, known as kerogen, which is the source of hydrocarbon generation. Its characterization and quantification are of paramount importance for evaluating potential productivity and the type of recoverable hydrocarbon. In this talk, we discuss two main issues: the characterization of kerogen maturity, which is an indicator of the production window, which may correspond to oil, gas, or an intermediate phase known as condensate. Rapid methods based on ^{1}H detection are compared with traditional ^{13}C CPMAS measurements. Another technique that is fundamental in the petroleum industry is the determination of fluids contained within the rock; for this purpose, the industry standard involves the use of equipment operating at magnetic fields of 0.05 - 0.5 T. We will present results to overcome limitations for probing both solid and liquid components in shale rocks.

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Diffusion coefficient measurements for moving samples under strong magnetic field gradients

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Among the numerous measurements carried out during a well-logging procedure, the Nuclear Magnetic Resonance (NMR) assessment is a fundamental analysis for determining the economic viability of a well for the oil industry. [1] Nowadays, two reliable approaches, Wireline Logging (WL) and Logging While Drilling (LWD), stand out. WL comprises the acquisition of NMR data under static conditions. On the other hand, in LWD, NMR measurements occur simultaneously with drilling, while the NMR tool experiences translation, rotation, and vibration relative to the rock formation. To better understand the NMR response acquired under LWD conditions, a setup emulating an LWD tool was developed, consisting of a single-sided magnet, radiofrequency probes, and a mechanical device that simulates relative sinusoidal motion between the sample and the applied magnetic field. [2] A bulk sample and three representative rocks, Fontainebleau Sandstone, Berea Sandstone, and Indiana Limestone, were investigated. Even though diffusion coefficient measurements are often neglected due to their inherent data-acquisition characteristics, the findings demonstrate that the diffusion coefficient of a fluid in a bulk sample or confined in a porous rock can be precisely measured and accurately predicted. [3] In strong magnetic field gradients, the Hahn spin echo is predominantly weighted by diffusion, an effect used to measure diffusion coefficients. Under LWD conditions, the diffusion coefficient measurement is significantly affected by signal phase modulation caused by sample movement in the presence of strong magnetic field gradients, making this measurement difficult. These results present solutions for accurate diffusion coefficient measurements by synchronizing Hahn spin-echo experiments with sample movement.

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Dipolar-Based Low-Field TD-NMR: From Soft Matter to Porous Media

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Low-field Time-Domain Nuclear Magnetic Resonance (TD-NMR) has become an important experimental approach for a wide variety of applications [1]. Continuous developments in instrumentation and methodology have substantially expanded its capabilities through the exploration of relaxation and diffusion phenomena, as well as changes in NMR interactions, such as dipolar couplings. As a result, TD-NMR is now widely employed for the characterization of material properties in a broad range of systems, including solids, soft materials, and porous media.

In ^{1}H TD-NMR studies of solid and soft materials, through-space magnetic dipolar couplings between ^{1}H nuclear spins play a crucial role, rendering the NMR signals highly sensitive to molecular packing and molecular mobility. This intrinsic sensitivity makes ^{1}H TD-NMR especially effective for identifying mobility transitions, including segmental motions in soft materials [2], freezing and melting phase transitions [3], and the dissolution of solids.

In this presentation, we explore the use of dipolar-based low-field TD-NMR methods across different classes of materials, ranging from soft matter to porous systems. Particular emphasis is placed on approaches based on dipolar filtering combined with the Magic Sandwich Echo (MSE) sequence and their applications to the characterization of molecular mobility in soft materials, water populations in cementitious materials, mesoporous structures by NMR cryoporometry, and solid dissolution processes in soils.

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EPR and DNP-MRI of Sandstones

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Electron paramagnetic resonance (EPR) of natural rock samples has been proposed for geological dating based on radioactive dosage in the subsurface creating defects in quartz. Quartz is the predominant component of sandstone (> 90 %) and can occupy a large fraction in granites (*ca*. 30 – 50 %); the high quantity of quartz makes the sensitive EPR of silica-centered radicals (E′) well-suited for measuring these effects. However, it is well known from recent chemical literature that mechanical impact on quartz powders also forms E′ centers (*e.g*., ball milling, tumbling, grinding, etc.). Therefore, stable E′ centers may form in quartz-rich geologic formations by tectonic and tidal deformations, or induced by human activities like tunneling, mining, and geoenergy applications. Herein, I will present results from laboratory-scale experiments of stress-induced microfracturing in Berea sandstones. Samples are subject to compressive and tensile loading or heating to induce microcracks, then analyzed by conventional CW X-band EPR and show the onset of additional E′ signals.

Furthermore, we explore using Overhauser dynamic nuclear polarization (ODNP) for enhancing ^{1}H signals in H_2O-saturated Berea sandstones. A homebuilt magnet and DNP-NMR apparatus is used based on inexpensive ferrite permanent magnets and a simple birdcage-style DNP resonator, respectively. Experiments are performed at approximately 50 mT, 2.1 MHz, and 1.4 GHz corresponding to the B_0 field, NMR frequency, and EPR/DNP frequency, respectively. Preliminary results show that the spin polarization is modulated according to DNP irradiation times and relative pore sizes. Consideration is given to using E′ in natural rock samples as an endogenous source of radicals for ODNP. Finally, a unique mechanism is revealed showing how hyperfine couplings can be spatially encoded into NMR spectra when ODNP is performed in a constant gradient field.

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Fluid transfers through versatile dynamic NMR relaxometry

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For years, our group has been developing innovative experimental methodologies [1] to monitor liquid transfer in porous media and complex fluids using dynamic NMR relaxometry. Combined with MRI, this non-invasive, multiscale, and time-resolved approach enables the individual tracking of all out-of-equilibrium protonic liquid phases during processes such as drying, imbibition, or internal water redistribution in model nanoporous media, for various applications involving geo-based (clay, granular systems) or bio-based materials (wood, paper, plant fibers [2]) and gels [3]. Here, we show how in this context, original quantitative information can be extracted from the detailed analysis of the evolution of the transverse NMR relaxation time distributions over time during such transfers based on fast exchange concept between bulk and surface water at the pore scale. Dynamic NMR relaxometry is able to reveal phenomena such as wetting and dewetting, chemical instabilities of the solid matrix, or the progressive loss of moisture homogeneity inside non-transparent materials — information that is highly valuable for improving predictive physical models of liquid transport for a large range of scale corresponding to all liquid states. Several examples of porous material and complex fluid will be presented to illustrate the versatility and robustness of this approach.

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Frequency domain NMR Relaxometry: the relevance of time scale and noise in data fitting

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The extraction of physical information from any experiment relies on two unavoidable and intimately connected essential aspects: the experiment itself and data processing [1]. The former pertains to both the hardware specifications and the experimental protocol that defines the measurement quality, whereas the latter is only meaningful when supported by a validated physical model or, alternatively, by carefully constrained model-free approaches.

In the context of frequency-domain NMR relaxometry, the fast field-cycling (FFC) technique [2,3] offers clear and well-established advantages over other methodologies, such as rotating-frame relaxometry. A key strength of FFC lies in the exceptionally broad range of Larmor frequencies that can be accessed through controlled cycling of the static magnetic field B0. Depending on the instrumental implementation, this approach enables the exploration of Larmor frequency windows spanning several orders of magnitude in the laboratory-frame. Moreover, both the fastest and slowest relaxation processes that can be probed also depend on the associated instrumentation.

In this contribution, we briefly discuss an illustrative example in which a single FFC NMR experiment enables the simultaneous estimation of the elastic bending modulus of liposome membranes and the diffusion dynamics of their constituent lipid molecules. This case study highlights the critical interplay between the experimental design, the model-based data analysis and the pertinence of the used fitting engine. We conclude by briefly commenting on the broader implications of these considerations for FFC NMR relaxometry studies in porous media.

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Localization-driven exchange contrast in diffusion exchange spectroscopy

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Diffusion exchange spectroscopy (DEXSY) is commonly interpreted using models that assume Gaussian diffusion within compartments and first-order exchange between them. Here, we show that DEXSY signal contrast with mixing time can arise even in the absence of barrier permeation. Specifically, a one-dimensional restricted domain with reflecting boundaries produces apparent exchange under strong-gradient conditions associated with signal localization (also known as "edge enhancement").

We consider DEXSY with identical, extended-gradient encodings. Signals were generated via a numerical approach that solves the Bloch-Torrey equation in discrete space and time using matrix operators. In the localization regime, spatially localized magnetization near boundaries redistributes during the mixing time, producing signal contrast that resembles first-order exchange. Fitting these signals with conventional exchange models yields an apparent first-order rate constant, k, despite the absence of first-order exchange.

The measured rate constant scales approximately as D/L^2, where D is the diffusivity and L is the domain size, with $k \approx \pi^2 D/L^2$ in many cases. We show that this behavior originates from the relaxation of *spatial* magnetization eigenmodes during the mixing time rather than transfer between distinct compartments; notably, $\pi^2 D/L^2$ is the first non-zero Laplacian eigenvalue for the restricted domain. We further identify the encoding and microstructural regimes in which this localization-driven exchange mechanism is expected.

These results demonstrate that DEXSY and related methods such as filter exchange spectroscopy (FEXSY) are not necessarily specific to genuine permeation across barriers. At the same time, the observed contrast provides sensitivity to the dominant spatial eigenmode(s) of restricted domains, suggesting a complementary source of microstructural information that may be obtained from such methods.

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Low-Field NMR Relaxometry System Solutions: Rapid Quantification of Pore and Fluid Properties in Porous Media

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Niumag has developed a fully integrated low-field NMR technology platform with independent intellectual property rights, covering single-board spectrometers, fast-discharge RF technology, in-house magnet manufacturing, and multidimensional relaxometry and imaging measurement technologies. This platform supports a systematic standard equipment portfolio for routine and advanced porous media analysis. The standard product portfolio includes benchtop analyzers for plug and cuttings samples, floor-standing analyzers for full-diameter cores, imaging analyzers for spatial fluid visualization, and modular relaxometers for T1/T2 and T1-T2 measurements. Standard configurations support multiple field strengths, open-bore and closed-bore magnets, and sample sizes from small plugs to full-diameter cores. All standard systems share a unified software platform for automated acquisition of FID/CPMG and other sequences, relaxation inversion, and petrophysical parameter calculation. Typical applications include porosity, permeability, bound and free fluids, movable fluids, and pore size distribution. Optional modules add temperature control, pressure capability, and fluid displacement, extending routine core analysis to reservoir-relevant conditions.

_eyond standard products, Niumag offers professional customization capabilities. Typical examples include: 1) multi-physics coupling NMR measurement systems for enhanced oil recovery (EOR) and flow-in-porous-media studies under complex stress, temperature, and pressure fields; and 2) field mobile NMR measurement systems for rapid on-site measurement and in-situ evaluation. These solutions bridge the gap between laboratory analysis and field applications, advancing low-field NMR as a mainstream quantitative method for porous media.

Magnetic Resonance Pore Imaging with Extended Echo Times and Cartesian q-Space Mapping

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Magnetic Resonance Pore Imaging (MRPI) also known as Diffusion Pore Imaging (DPI) [1] provides information on the structure of porous media by the acquisition of averaged pore shapes. The technique builds upon the pulsed-gradient spin-echo (PGSE) concept, but extends one diffusion-encoding gradient so that, in the long-time limit, the measured signal $E(q)$ approaches the pore form factor $S_0(q)$. This approach, inherently based on q-space, can also be combined with conventional k-space MRI, resulting in MRPI mapping [2].

A requirement for MRPI is the need for long echo times. This can be challenging experimentally because of relaxation decays, gradient imbalance, or gradient-induced dephasing [3]. Recently, we have shown that, under favourable conditions and in specific geometries, spin echo times (TE) can be pushed to approximately 2 s [EUROMAR 2025].

Here, we deploy these extended echo times to re-implement 1D and 2D PGSE/MRPI experiments in glass capillaries while retaining high signal-to-noise ratios using a simple spin-echo acquisition rather than a CPMG-backbone MRPI sequence as used previously [2]. In 1D PGSE, diffusive-diffraction minima remained visible with good SNR to echo times of up 500 ms while in 1D MRPI, echo times reached up to 800 ms, improving convergence of $E(q)$ towards $S_0(q)$

In 2D MRPI, a Cartesian q-space sampling scheme was used in conjunction with echo times of up to 400 ms. These yielded suitable cross-sectional pore-shape reconstructions from the capillary bundles. We are currently extending this 2D MRPI approach towards mapping, retaining the 2D Cartesian q-space scheme while combining it with a Cartesian k-space scheme. This will allow 2D pore images to be reconstructed by Fourier transformation only, providing a route towards spatially resolved 2D×2D MRPI, where different pore-size populations within the same sample can be separated while retaining the simplicity of a single spin-echo acquisition.

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Robust Methods and Durable Devices for NMR in Harsh, Non-laboratory Conditions

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Non-laboratory, at the point – of – care, field measurements require more than personnel and instruments. Most commercially available NMR instruments are not durable enough to survive deployment to real, harsh factory conditions involving severe electronic noise, mechanical vibration, and an uncontrolled environment. Also, these real non-laboratory conditions, unfamiliar to most spectroscopists, make most data acquisition and processing protocols unstable. Examples of stable data processing methods, portable lightweight, inexpensive instruments and their use in factories, the outdoors and hotel rooms will be provided and used to highlight the steps needed to convert real field measurements into meaningful information.

Understanding NMR Signal Behavior Under Sample Motion: Implications for Logging While Drilling Operations

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Logging While Drilling (LWD) NMR measurements are critical for in-situ petrophysical characterization. Although mathematical correction approaches have been proposed to account for sample motion effects on transverse relaxation (T_2) measurements [1, 2], the comprehensive applicability of these corrections remains incompletely understood. This study investigates the effects of mechanical oscillations on NMR signals in representative rock samples using a laboratory-scale LWD emulator. Four different samples—three sandstones (Fontainebleau, Berea, Portland Red) and one carbonate (Indiana Limestone)—covering a broad range of relaxation times were analyzed under controlled sinusoidal motion at frequencies from 1–4 Hz and amplitudes up to 5 mm. Results demonstrate that sample motion significantly alters relaxation time distributions and pore size distribution interpretations, particularly when T_2 values are comparable to oscillation periods. However, crucially, total porosity estimates remain robust and independent of sample motion across all conditions, including high-amplitude oscillations. These findings reconcile contradictions in the literature regarding porosity loss during LWD operations and provide critical insights for improving petrophysical interpretation models in dynamic drilling environments. This work establishes practical guidelines for field data acquisition and processing under complex motion scenarios in the oil and gas industry.

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Magnetic Resonance in Porous Media 2026

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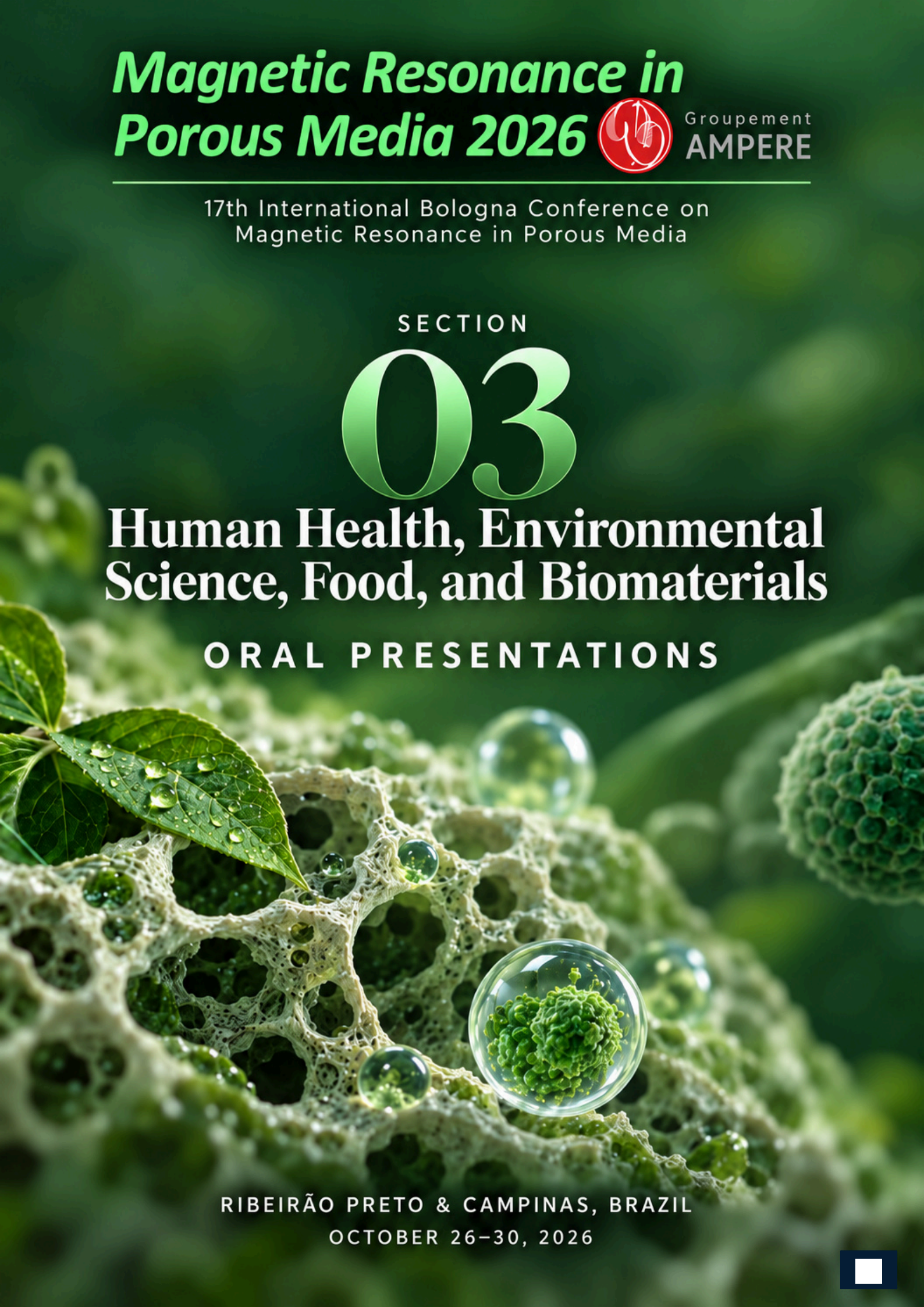
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SECTION

03

Human Health, Environmental Science, Food, and Biomaterials

ORAL PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

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A Low-Field MRI scanner for Multimodal Preclinical Imaging: Gamma detected-MRI

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The GAMMA-MRI project [1] explores magnetic-resonance spatial encoding of gamma photons emitted by hyperpolarized xenon isomers, detected by gamma sensors surrounding the subject [2]. This approach may achieve sensitivity to about 10^{13} spins while retaining the adaptability and spatial resolution of conventional MRI while working at low magnetic field.

Low-field MRI is gaining attention due to advances in permanent magnets and electronics, offering portability, lower acquisition and maintenance costs, improved sustainability, and flexibility for application-specific designs and multimodal integration.

We present principles and examples of custom MR instrumentation [3], focusing on a low-field preclinical scanner developed for small-animal imaging. To preserve access for GAMMA-MRI detection, the system uses a yokeless C-shaped permanent magnet with a central bore and 160 mm pole gap. The compact, portable assembly weighs about 40 kg and produces a 50 mT field; its homogeneity and temporal stability are characterized. Custom gradient coils and second-order shim elements were designed to maintain bore access. Initial proton images of phantoms were acquired using inductive Faraday detection and reconstructed with conventional PFG Fourier methods and alternative inverse Laplace/Radon techniques. Sensitivity and spatial resolution in standard operation are reported. Ongoing work targets full integration and in vivo imaging.

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Characterization of 3D-Printed Biomimetic Scaffolds by Low-Field NMR: Relaxation and Diffusion Studies in Soft Porous Media

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The design of effective 3D-printed biomimetic scaffolds, such as collagen-hyaluronic acid hydrogels, requires rigorous characterization of their hierarchical pore networks and fluid-matrix interactions. Standard imaging techniques require drying and are destructive, failing to capture the physical reality of soft porous materials in their fully hydrated, functional state. This study presents a low-field Nuclear Magnetic Resonance (LF-NMR) methodology to characterize the hierarchical porosity, water dynamics, and structural anisotropy of these soft porous media subjected to different crosslinking treatments (physical or chemical). In particular, the focus is on the effect of crosslinking on water dynamics, pore network characterization, and microstructural anisotropy.

Transverse relaxation times showed distinct water populations representing different hierarchically confined pore environments. Porosity was also evaluated, linking crosslinking density to the swelling capacity of the network. Two-dimensional T_1-T_2 correlation maps were used to evaluate exchange kinetics and confinement mechanisms at the biopolymer-solvent interface. The resulting deviations from the free-water diagonal directly revealed changes in the segment mobility of the polymer chains. Furthermore, the Magic Angle effect was exploited using the Magic Sandwich Echo (MSE-FID) sequence in the frequency domain to assess microstructural anisotropy of the material fibers induced by shear stresses during printing extrusion and its subsequent crosslinking. Additionally, components of the diffusion tensor were investigated using a unilateral NMR-MOUSE sensor to quantify directional mass transport within the scaffold matrices. The combination of these LF-NMR techniques provides a direct, non-destructive framework to quantify the physical properties and transport dynamics of soft porous biomaterials.

Acknowledgements

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Climate change: the science, impacts, and mitigation strategies

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Fossil fuel use largely drives climate change by increasing greenhouse gas emissions. Rising temperatures are changing weather patterns and intensifying extreme climate events. These shifts affect ecosystems, agriculture, water supplies, and human health. The impacts are uneven, placing greater burdens on vulnerable communities. Climate science helps explain these changes and project future risks. Reducing emissions is essential to limit further warming. Key strategies include clean energy, energy efficiency, and sustainable transport. Protecting forests and restoring ecosystems can also absorb carbon. Adaptation measures help communities prepare for unavoidable impacts. Combining mitigation with adaptation is crucial in building a new sustainable society

CNPEM, a Unique Laboratory in Latin America

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The Brazilian Center for Research in Energy and Materials (CNPEM) is a cutting-edge, multi-user, multidisciplinary scientific environment that supports the Brazilian National Science, Technology and Innovation System. It has globally competitive laboratory infrastructures open to the scientific community, such as Sirius, one of the world´s most advanced synchrotron light source. The Center combines a range of skills, with an emphasis on nanotechnology, biosciences, biotechnology, biorenewables, cutting-edge engineering and scientific instrumentation, carrying out research and development in strategic areas such as health, energy, renewable materials, and sustainability, including innovative projects in partnership with the productive sector and contributing to the training of researchers and students. The Center is also responsible for the Ilum School of Science, a higher education course in Science, Technology and Innovation. CNPEM has recently began developing the Orion project, a laboratory complex for advanced research in pathogens, which will host facilities with advanced levels of biological containment (BSL-3 and BSL-4), planned to be the first in the world to be connected to a synchrotron light source. In this seminar an overview of the CNPEM's activities will be presented.

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https://cnpem.br/

CO_2 Storage Strategies in the Oil Sector – Perspectives in Petrobras

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Evaluating porous media for Carbon Capture and Storage (CCS) requires a fundamental shift from traditional petroleum reservoir engineering frameworks. While oil and gas characterization primarily focuses on hydrocarbon recovery, CCS demands a comprehensive understanding of long-term containment, multi-phase fluid-rock interactions, and complex trapping mechanisms over geological timescales. This presentation addresses fundamental aspects of geological CO2 storage, focusing on designing reliable Measurement, Monitoring, and Verification (MMV) programs. In this context, we give an overview of well monitoring technologies and strategies to be tested in Petrobras pilot-scale MMV of Barra do Furado, which will also include a sensitivity analysis of time-lapse NMR well logging.

Determining the Crystallite Size of Organic Solids with ^{1}H NMR T_1 Relaxation

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Polycrystalline organic solids are ubiquitous in food, pharmaceutical, and chemical industries. We demonstrate that the ^{1}H T_1 relaxation time of polycrystalline organic solids is strongly correlated with crystallite size over more than four orders of magnitude in size, from approximately 50 nm to 1 mm. We explain this behavior through a relaxation-diffusion model in which nuclear magnetization first migrates from the crystal interior to the surface by spin diffusion and subsequently relaxes at surface sinks. Therefore, larger crystals have a longer spin-diffusion length and hence longer T_1 relaxation time. This mechanism is analogous to the NMR relaxation of liquids in porous materials, where mass diffusion to relaxing surfaces produces relaxation times that are correlated to the pore size. We present evidence from literature data, model systems, commercial pharmaceutical lactose powders, and lactose tablets compressed at different tableting pressures. The model shows two distinct regimes corresponding to fast and slow spin diffusion and explains both linear and quadratic scaling relationships between ^{1}H T_1 and crystallite size. In low-temperature and dynamic nuclear polarization data, we observed nonground relaxation eigenmodes and used them to estimate the absolute crystallite size. Our findings establish ^{1}H T_1 relaxation as a non-invasive probe of crystallite size and suggest applications in the characterization and process monitoring of pharmaceutical, food, agricultural, and chemical materials.

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Diffusion Dynamics in Axons and the understanding of diffusion MRI in Brain

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Diffusion MRI is widely used for the clinical examination of a variety of diseases of the nervous system. However, clinical MRI scanners are mostly capable of low magnetic field gradients. The availability of the Connectome MRI scanners with ultra-high gradient strengths up to 300 mT/m enables the resolution of a wider range of diffusion coefficients and tissue structures. In addition, biological tissues are heterogeneous on many scales and the complexity of tissue microstructure may not be accurately captured by simplistic models based on pre-existing assumptions. For example, an axon may not be considered as a straight tube as in most of the diffusion literature. Here, we study the intrinsic diffusion physics in thousands of realistic axon models and show a diversity of diffusion behavior. We outline a framework for analyzing diffusion MRI to obtain a model-free Full Diffusion Tensor Distribution (FDTD). We then apply this method and use a machine learning method to identify features in FDTD to visualize and characterize tissue heterogeneity in diffuse gliomas.

Diffusion MRI in cerebral small vessel disease: characterization of longitudinal microstructural decline with advanced markers

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Cerebral small vessel disease (cSVD) is an umbrella term used to collectively describe different pathologies that affect small blood vessels in the brain. It's an emerging disease, contributing to 45% of dementia and 25% of stroke cases worldwide [1]. Diffusion MRI (dMRI) parameters have shown larger sensitivity to disease severity and progression compared to conventional markers based on structural MRI, such as white matter hyperintensities and microbleeds [2]. This work aimed to investigate whether these dMRI metrics can detect longitudinal decline in SVD patients. A cohort of 48 SVD patients was identified on the UK Biobank (application ID: 155020), with median age at baseline of 69 years (IQR: 66-74 years) and median follow-up time of 2.23 years (IQR: 2.07-2.28 years). DTI (Diffusion Tensor Imaging) and NODDI (Neurite Orientation and Density Imaging) model parameters were extracted in white matter (WM) and grey matter (GM) ROIs. Linear mixed-effects models were employed to study longitudinal change of the parameters in each ROI, adjusting for baseline age and sex and applying FDR correction. Significant differences ($p<0.05$) were found across several WM ROIs, most notably in the corona radiata, internal and external capsules, corpus callosum, and superior longitudinal fasciculus (effect sizes 0.1-0.2 sd/year). These results highlight the sensitivity of advanced dMRI metrics to WM longitudinal deterioration in cSVD. Future work will explore the relationship between these metrics and cognitive performance, to further validate the clinical importance of these biomarkers.

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Low-Field NMR Relaxometry for GAG Assessment: A Multimodal Investigation of Articular Cartilage

Leonardo Conti[1], Simone Fantoni[2], Matteo Berni[2], Carola Cavallo[3], Roberta Fognani[2], Paolo Cardarelli[4], Claudia Testa[1], Fabio Baruffaldi[2], Leonardo Brizi[1]

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Articular cartilage (AC) is a soft tissue covering the extremities of articulating bones within synovial joints. The collagen mesh, intertwined proteoglycans (PG) and their associated glycosaminoglycan (GAG) chains form a heterogeneous pore structure that constrains interstitial water. Single-sided Nuclear Magnetic Resonance (SS-NMR) relaxometry has been shown to discriminate tissue composition and structure among the three AC zones[1]. This work investigated the sensitivity of SS-NMR to GAG concentration by comparing T_1 and T_2 distributions against results from contrast-enhanced µCT, used as a reference technique. To further establish a multidisciplinary framework linking AC composition, structure, and mechanics, the relationship between NMR parameters and tissue mechanical properties was explored via indentation testing.

Thirty-two osteochondral samples were retrieved from the knee joints of healthy bovines. After indentation testing[2], CPMG and Saturation Recovery measurements were performed for each of the AC zones using an NMR-MOUSE (B_0=0.327 T) device. Finally, samples were exposed to CA4+, a cationic contrast agent affine to GAG chains[3], and imaged with a tabletop µCT system. The CT reference procedure was further validated via biochemical assay. Descriptive statistics of T_1 and T_2 distributions obtained using the UPEN algorithm were compared with the average CT attenuation coefficient for each zone and the samples' mechanical parameters.

Preliminary results showed a positive relationship between CT attenuation and the signal fraction of the short T_2 component (0.1–5 ms; Spearman ρ=0.54) as well as an inverse trend with its full width at half maximum (FWHM,ρ=-0.54). In addition, the FWHM of the T_1 distribution showed an inverse relationship with the timescale of the viscoelastic response (ρ=-0.67). These findings support the role of GAG chains in water confinement and suggest SS-NMR as a useful technique for probing AC composition and mechanical properties.

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Magnetic Resonance and Magnetic Resonance Imaging with a Variable Field Cryogen Free Superconducting Magnet

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Magnetic Resonance of realistic materials is often confounded by magnetic susceptibility mismatch effects which dramatically increase the MR linewidth. In an ideal world one would wish to choose the maximum field strength (for more signal) consistent with a tolerable magnetic susceptibility mis match effect. For several years we have been employing a cryogen free magnet with an integrated magnet power supply which permits us to increase or decrease the static field as desired, controlling linewidth and susceptibility effects for relaxation and imaging studies.

There is however another advantage of the variable field magnet approach to materials MR/MRI. If we are studying a system with a complicated apparatus (for example a battery or a system at high temperature and pressure) the simplest possible RF probe is desirable. The variable field magnet makes it possible to bring different nuclei into resonance while maintain the original resonance frequency. The RF probe in this case maintains a constant frequency and constant sensitivity even as we change the nuceli being interrogated. For example, at 0.79 T the 1H frequency is 33 MHz. If the field is increased to 2.99 T we measure 23Na at 33 MHz and if we increase the field to 3.1 Tesla we measure 13C at 33 MHz.

In this presentation we will outline measurements where we adjust the field to control susceptibility mismatch effects, and we will describe measurements in systems where we adopt the field changing approach to undertake 19F, 13C, 23Na and 7Li studies in conjunction with 1H for battery studies and studies of fluids in porous media.

The Pore Size of PLGA Bone Implants Determines the De Novo Formation of Bone Tissue in Tibial Head Defects in Rats

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Purpose: The influence of the pore size of biodegradable poly(lactic-co-glycolic acid) scaffolds on bone regeneration was investigated.
Methods: Cylindrical poly(lactic-co-glycolic acid) scaffolds were implanted into a defect in the tibial head of rats. Pore sizes of 100–300, 300–500, and 500–710 µm were tested and compared to untreated defects as control. Two and four weeks after implantation, the specimens were explanted and defect regeneration and de novo extracellular matrix generation were investigated by MRI, quantitative solid-state NMR, and mass spectrometry.
Results: The pore size of the scaffolds had a pronounced influence on the quantity of the extracellular matrix synthesized in the graft; most collagen was synthesized within the first 2 weeks of implantation, while the amount of hydroxyapatite increased in the second 2 weeks. After 4 weeks, the scaffolds contained large quantities of newly formed lamellar bone while the control defects were filled by inhomogenous woven bone.
Best results were obtained for scaffolds of a pore size of 300–500 µm.
Conclusion: Our analysis showed that the structure and dynamics of the regenerated extracellular matrix was very similar to that of the native bone, suggesting that biomineralization was significantly enhanced by the choice of the most appropriate implant material.

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SECTION

04

Natural and Artificial Porous Media & Cultural Heritage

ORAL PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL
OCTOBER 26–30, 2026

Application of Proton Time-Domain NMR to Investigate Water Distribution and Pore Structure Development in Low-Carbon Cements

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Proton Time-Domain Nuclear Magnetic Resonance (^{1}H TD-NMR) was applied to investigate the role of water in low-carbon cements containing calcined clay, both in the fresh and hardened state. Water distribution in cement pastes was studied using transverse, T_2, relaxation times acquired with Carr–Purcell–Meiboom–Gill (CPMG) sequences. It is shown that the intraparticle pores of calcined clay particles absorb a significant fraction of the mixing water, reducing the amount of free water available in the system. This phenomenon affects the rheological behavior of fresh binders and may explain the loss of workability commonly observed in calcined clay-based cements.

Furthermore, Logarithmic Aperiodic Pulse Saturation Recovery (LAPSR) experiments and two-dimensional T_1–T_2 relaxation maps were used to follow the evolution of water environments during hydration. The NMR signals were processed through quasi-continuous linear 1D and 2D inversion using the software packages UPENWin and MUPEN2D, respectively, allowing the reconstruction of one- and two-dimensional relaxation time distributions. The analysis provided information on water mobility, pore structure refinement and the progressive development of hydration products.

In particular, white Portland cement, ordinary Portland cement and limestone calcined clay cement were investigated, and they showed distinct relaxation behavior, with T_1/T_2 ratios of approximately 2.5, 2.0 and 1.5, respectively. Relaxation behavior revealed differences in water–surface interactions and pore structure evolution during hydration, with iron-bearing phases affecting microstructural development but not significantly altering interlayer water relaxation.

The combined use of TD-NMR relaxation time distributions and T1–T2 correlation maps enabled the characterization of water dynamics and pore structure evolution during hydration of low-carbon cementitious systems.

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Capabilities of the Powder X-ray Diffraction Beamline (PAINEIRA) at SIRIUS for Structural Characterization of Porous Materials

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X-ray diffraction analysis of polycrystals (PXRD) is crucial for examining the correlation between the crystalline structure and porosity and, consequently, its functionality. The organized packing of atoms and molecules dictates the size, shape, and connectivity of the void spaces that form, and this relationship is essential in material science and engineering. The Powder X-ray Diffraction technique using synchrotron radiation (SR-PXRD) offers advantages such as high photon flux, low-divergence X-ray beams, and adjustable energy levels, thereby minimizing instrumental effects on peak profiles and enabling high-resolution analyses. The PAINEIRA beamline is a facility dedicated to X-ray diffraction characterization of polycrystalline materials at the Brazilian synchrotron radiation (SR) facility, SIRIUS [1]. The benefits of using SR-XRD for characterizing polycrystalline materials at PAINEIRA extend beyond high resolution and signal-to-noise ratio. SR-XRD experiments can be combined with appropriate sample environments, fluid-handling systems, and large angular resolution and fast detectors to facilitate in situ and operando experiments that reveal transient crystalline phases or structures responsible for the performance of functional materials [2]. The beamline was designed to be efficient and flexible for data acquisition, providing high angular resolution with a multi-analyzer crystal detector and/or a fast-area detector. Automated experiments under variable temperature conditions will also be available [2]. In this presentation, I will provide an overview of the PAINEIRA beamline, primarily focusing on the mechanical, automated, and computational tools [3] that enhance efficiency and create a user-friendly environment for powder X-ray diffraction experiments. Ultimately, it will be demonstrated how this specialized synchrotron tool can investigate fundamental material properties at the atomic level and correlate them with their corresponding functions.

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Characterization of magnetic rocks: a challenge for NMR

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Mapping mineral and pore distributions across scales is crucial for evaluating geochemical and reactive transport properties of subsurface rocks that underlie subsurface applications such as, oil and gas production, geological carbon storage/mineralization, geologic hydrogen generation, and mining exploration. Many of the relevant rocks contain a high percentage of iron and magnetic minerals so that the NMR relaxation is strongly affected by diffusion in the internal magnetic fields, even for very short echo times. Furthermore, the internal fields and their gradients are heterogeneous among the different pores, making it difficult to obtain the intrinsic T2. We developed a new pulse sequence to separate the diffusion and intrinsic relaxation effects and recover the intrinsic T2 for pore size determination. We have also developed a method for high-throughput super-resolution mineralogy mapping based on SEM imaging to identify the fine grain minerals for multiscale characterizations of rock mineralogy from submicron to centimeters. We will report our results on basalt, sandstone, carbonate and other mine rock samples. These new methods could be beneficial for a wide range of subsurface exploration.

Combined quantitative ^{1}H, ^{23}Na and ^{35}Cl NMR to study the salt crystallization of NaCl–NaNO3 mixtures in sandstone during drying

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Salt crystallization is one of the major causes of deterioration of cultural heritage objects. While most studies focus on the crystallization behaviour of single salts real heritage materials are commonly exposed to complex salt mixtures. These mixtures are problematic due to their complex interactions and the crystallization is usually interpreted using equilibrium phase diagrams.

In this study, we investigate the crystallization behaviour of NaCl–$NaNO_3$ mixtures during drying in sandstone using a dedicated 4.7 T NMR setup. Quantitative measurements of ^{1}H, ^{23}Na and ^{35}Cl signals were performed quasi-simultaneously, allowing the determine the ratio of NaCl-$NaNO_3$ remaining in solution throughout the drying process. Hence the evolution of the salt mixture ratio can be monitored directly, providing direct insight into the crystallization pathway.

The sandstone samples were saturated with solutions containing different NaCl–$NaNO_3$ ratios and subsequently dried. Analysis of the drying curves yielded Peclet numbers between 5 and 10, indicating that ion transport is dominated by advection. The NMR measurements reveal that the ratio of NaCl-$NaNO_3$ in solution remains essentially constant throughout drying for all investigated mixtures. This behaviour is in sharp contrast to predictions based on equilibrium phase diagram, which anticipate substantial changes in solution composition.

The results indicate that under drying conditions crystallization is essentially transport-driven. The commonly used equilibrium approximation is therefore insufficient to describe salt-mixture crystallization. Indeed, this NMR study reveals that the equilibrium approximation does not hold under drying conditions and the measurements seem to indicate that either NaCl or NaNO3 supersaturate, resulting the ratio keeping constant. These findings have important implications for understanding salt damage in cultural heritage and for interpreting salt analyses obtained from weathered porous materials.

Acknowledgements

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Development of Portland Cement Binders with Low CO_2 Footprint Utilizing Solid-State NMR spectroscopy

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Solid-state NMR, in particular ^{27}Al and ^{29}Si NMR, has been an invaluable tool for characterization of the structure, composition, and reactivity of Portland cement, supplementary cementitious materials (SCMs) such as calcined clays, and carbonation products [1]. This will be illustrated by three examples:
(i) For calcined clay - limestone Portland cements, ^{27}Al and ^{29}Si NMR has been provided information about the degree of reaction of the calcined clay (metakaolin) and the evolution of the Al-bearing phases during hydration. The principal binding phase is a less-ordered calcium-(alumino)-silicate-hydrate (C-(A)-S-H) phase, where the combi-nation of ^{27}Al and ^{29}Si NMR has provided quantitative information on Al in this phase, giving a more detailed picture on the capacity of the C-(A)-S-H phase to incorporate Al under different compositional conditions and at different hydration stages.
(ii) ^{27}Al and ^{29}Si NMR investigations of aqueous carbonation of Portland cement pastes, incorporating different types of SCMs, reveal that nearly all calcium-bearing phases can be carbonated and thereby, that the initial calcium content governs the CO_2 uptake capacity. A model for deconvolution of the ^{29}Si NMR spectra of the carbonated cement pastes has been established, which has led to a structural model for the alumina-silica gel that accounts for the Al/Si ratio and the degree of polymerization of the gel [2].
(iii) ^{1}H, ^{13}C, and ^{27}Al NMR experiments at very high magnetic field (22.3 T) has been utilized to characterize the structural environments for these elements in the cement hydrate phase, monocarbonate ($Ca_4Al_2(OH)_{12}(CO_3)\cdot 5H_2O$). Here, the combination of the very high magnetic field and ultra-fast MAS (ν_R = 100 kHz) has allowed resolution of the 22 distinct ^{1}H resonances in a ^{1}H–^{1}H SQ-DQ (BABA) MAS experiment. The ^{1}H resonances are assigned to distinct sites in the hydrogen network from the correlations in the 2D spectrum combined structural relations for 1H chemical shifts.

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Enhancing magnesium mineral carbonation in Western Australia for sustainable carbon storage

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The natural global carbon cycle has been overwhelmed by anthropogenic carbon emissions, resulting in rapid increase in atmospheric CO2. Secure long-term storage of this CO2 by mineral carbonation (*i.e.* reaction of CO2 with alkaline solids to form carbonates) is thermodynamically stable, and is the main source of long-term atmospheric cooling on the Earth via silicate weathering processes. It is possible to accelerate such mineral carbonation, but this is complicated by the economic costs, large volumes and long timeframes required for secure CO2 storage. The process of direct mineral carbonation has in the last decade been demonstrated at industrial scales (e.g. the CarbFix project in Iceland), however these processes typically require specific local geographical advantages. Western Australia (WA) is rich in mafic and ultramafic formations containing minerals critical to future renewable energy technologies, mining these results in large quantities of mafic (magnesium and iron rich) mine tailings. WA is also rich in acidic brine lakes and acidic groundwater networks with low pH, these natural acidic brine lakes are rare globally. These components offer opportunities for developing novel, lower cost mineral carbonation processes in WA to off-set CO2 production. The current project investigates the combination of acidic brine and mafic mine tailings to enhance the performance of magnesium-based mineral carbonation. An important component of this project is the non-invasive monitoring of the carbonation process using low field nuclear magnetic resonance (NMR), specifically the effect of exposed ferromagnetic surfaces on NMR signal relaxation, for the in-situ measurement of fractional surface coverage by the solid carbonate product. The critical balance between deposition rate and maximum access to, and use of, the tailings pore space can be dynamically probed and is important to assessing volumetric CO2 storage capacity.

Acknowledgements

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Monitoring the Hydration of Brazilian Commercial Cements Using Low-Field NMR

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Low-field Nuclear Magnetic Resonance (LF-NMR) is a rapid and non-destructive technique with the potential to assess cement reactivity by monitoring water evolution during hydration. This study evaluates the applicability of LF-NMR for monitoring the hydration of Brazilian commercial cements with different chemical compositions.

Six cements were investigated, including one white cement with negligible iron content and five gray cements containing different levels of iron oxide. Hydration was monitored using a SPEC FIT DC low-field NMR system operating at 20 MHz. The NMR results were compared with conventional techniques used to assess cement reactivity, namely isothermal calorimetry and chemically bound water measurements.

The evolution of the NMR signal showed good agreement with both cumulative heat release and chemically bound water, confirming the ability of LF-NMR to track hydration progress. Strong correlations were observed between NMR measurements and the independent hydration indicators, demonstrating the potential of the technique for evaluating the hydration kinetics of commercial cements.

However, differences in NMR signal intensity were observed among cements exhibiting similar hydration behavior according to calorimetry and bound water measurements. In addition, no direct correlation was found between the total iron oxide content measured by X-ray fluorescence (XRF) and the NMR signal intensity. These results suggest that the NMR response is influenced not only by the hydration degree but also by magnetic characteristics of the cement, possibly associated with magnetically active iron-bearing phases.

Overall, the results demonstrate that LF-NMR is a valuable tool for monitoring the hydration of commercial cements and highlight the importance of considering compositional effects when comparing NMR measurements obtained from different cement types.

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Reducing CO_2 Emissions in the Cement Industry

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Cement is the world's most produced artificial material, with annual demand of about 4.2 Gt (0.5 t per capita). Its production requires thermal decomposition of limestone, releasing chemically bound CO_2 and emissions from fuel combustion. Despite major efficiency improvements, cement manufacturing still accounts for roughly 6–8% of global anthropogenic CO_2 emissions.

Its environmental footprint extends beyond production. Cement is typically only 15% of the mass of concrete and mortar, making the resource footprint of cement-based materials about eight times larger than cement itself. These materials consume nearly 30% of all extracted natural resources and generate large volumes of long-lived construction waste.

Cement-based materials remain essential because raw materials are widely available, costs are low, and the technology is simple to use, even for untrained workers. These advantages are especially important in developing regions, where future demand will be concentrated.

With conventional mitigation options largely exhausted, the industry expects carbon capture and storage (CCS) to deliver about one-third of future emissions reductions. However, its high cost highlights the need for alternative, rapidly scalable solutions.

Cement consists mainly of CaO, SiO_2, Al_2O_3, and usually Fe_2O_3. It hardens through complex hydration reactions that form new mineral phases. Water is added primarily to achieve the required rheology and often exceeds stoichiometric needs. Excess water creates porosity, which strongly influences strength, stiffness, transport properties, and durability.

Nuclear Magnetic Resonance (NMR) is a valuable tool for monitoring hydration reactions and characterizing hydrated phases, pore volume, and pore-size distribution.

This presentation will discuss low-carbon, low-cost, easy-to-use cement technologies with potential for rapid large-scale deployment and highlight related research opportunities for the NMR community.

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Soil Pore Size Distribution and Water Retention Curves by Low-Field NMR

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Freshwater scarcity is a preeminent global challenge, with agriculture alone accounting for 70% of total consumption. Soil's capacity to retain water, filter solutes, and recharge aquifers is dictated by its **Soil Water Retention Curve (SWRC)** As a fundamental property in soil physics, the SWRC—alongside pore size distribution—is essential for modeling fluid and solute transport within the vadose zone. These properties have critical implications across agriculture, forestry, ecology, and civil engineering.

The Current Bottleneck Despite their importance, quantifying soil hydraulic properties remains a significant challenge. Conventional empirical methods, such as porous plates and pressure cells, are: **Laborious and time-consuming:** *Often taking weeks or months;* **Expensive:** *Requiring specialised, high-maintenance equipment;* **Prone to error:** *Susceptible to operator bias and experimental inaccuracies.*

These limitations make hydraulic characterisation the primary bottleneck in soil physics laboratories worldwide.

A New Analytical Frontier: NMR Relaxometry While ^{1}H NMR relaxometry has been used to characterise soil porosity, it often presents an "ill-posed problem." Traditional T_1 and T_2 results are confounded by two correlated unknowns: **pore length scales** and **surface relaxivity**.

To overcome this issue, we propose (Novotny et al., 2023) using a method that directly accesses **NMR diffusion modes**. This approach is governed solely by pore size, making it independent of unknown surface relaxivity. Our refined low-field NMR method is: **Fast:** *Delivers results in under 90 minutes;* **Precise:** *Provides unprecedented resolution and accuracy;* **Comprehensive:** *Simultaneously determines pore size distribution, the SWRC, and hydraulic conductivity.*

Validation and Results The results confirm that the proposed approach accurately determines pore size distribution and estimates SWRC in a fraction of the time required by conventional techniques.

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Soil Strategic Role in Global Food Production and CO2 emissions mitigation

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The soil, a very complex porous media, is the third bigger carbon reservoir of Planet, above of the atmosphere and biota pools sizes together, and with around less than half of Geologic pool, which is largely associated with increased greenhouse gas emissions (GHG) and climate change impacts. Besides to be an important carbon reservoir soil is pivotal to global agricultural sector that is one of few economic sectors that can work to reduce their own GHG emissions, using more sustainable practices, and simultaneously contribute to carbon sequestration, incorporated as a natural increase of soil organic matter content. So, in recent years soil has received a massive scientific effort to face adaptation and mitigation to global climate change challenges. In this presentation will be described a short overview of recent soil carbon scientific findings and combined with our research data of soil carbon sequestration from long term field experiments and large farms operations, and that includes innovative high and low field nuclear magnetic resonance results, demonstrating interesting achievements to conciliate agriculture and GHG emissions mitigation.

Magnetic Resonance in Porous Media 2026

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Magnetic Resonance in Porous Media

SECTION

05

Mobile NMR

ORAL PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

OCTOBER 26–30, 2026

3D printed passive shims for permanent magnets: Application to iron-pole, Halbach arrays, and a unique tilted field magnet

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Magnetically soft materials offer significant advantages over hard materials for implementing passive shims. In previous work, we have leveraged the ease of handling, the high precision and accuracy, and the low cost of magnetic ink to shim high-performance iron-pole magnets to sub ppm homogeneity.

For lower homogeneity magnets, for example those designed for time-domain measurements, the ink is not magnetically strong enough. For these magnets, we have been using 3D printed magnetic filament to achieve field improvements. We have found that readily available filament and a mid-level 3D printer are more than adequate for producing passive shims that substantially improve homogeneity. The precision is high enough that it is worthwhile to develop custom slicing software to drive the printer, thereby enabling improved accuracy in producing the calculated shim design.

We have applied 3D printed passive shims in a 0.3 T, 60 mm gap iron-pole magnet from Fine Instrument Technology (Brazil), reducing the peak-to-peak field variation over a 40 mm diameter sphere from 570 to 220 ppm. The final field error is almost entirely due to a Z^6 field, which is of high enough mathematical order that it has minimal impact on the NMR signal.

Halbach array/ring magnets can also be shimmed this way. For two magnets with 40 mm bores, we have achieved improvement over a 40 mm diameter sphere from 5625 to 221 ppm at 0.5 T and 400 to 14 ppm at 1.4T.

Presently, we are applying our methods to a 0.08 T cylindrical magnet from RE Magnet Studio, Ltd. that has a field pointing at 54.7 degrees with respect to the cylinder axis. We discuss the challenges of designing shims for such a magnet and (time permitting) the resulting homogeneity improvement.

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Compact and Mobile NMR

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The beginnings of compact NMR can be traced to the introduction of tabletop relaxometers for food quality control and materials testing in the early 1970ies. Mobile NMR started even earlier in the 1950ies with the exploration of earth-field NMR for well logging. It received a decisive boost with the introduction of permanent magnets in 1980, which enabled the sensitive volume to be localized in the stray field of the magnet. A derivative of this development are small stray-field devices for materials testing, one of which is the NMR-MOUSE. Efforts to shape the stray magnetic field benefitted the development of compact centerfield magnets for benchtop NMR spectroscopy with fields sufficiently homogeneous to resolve the chemical shift of protons in liquids. Miniaturizing the electronics and the magnet even further pushes the application of handheld centerfield relaxometers and miniature magnetic resonance sensors. Such sensors are particularly useful for rapid testing of short-lived and degradable products. The development of compact and mobile NMR is reviewed wit attention to current developments and concluded with a recent study of an antique, late-Roman burial chamber in Trier, where moisture flux towards the surface of a naturally wet wall has been estimated based on NMR depth profiles and Fick's first law.

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Drug-Assisted Network Formation in Biopolymeric Wound Dressing Membranes Revealed by Single-Sided and Benchtop NMR

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Burn wound dressings based on hydrophilic biopolymers require controlled network formation for adequate structural properties and drug retention. Although ionic crosslinkers are commonly used, the role of active pharmaceutical ingredients (APIs) in membrane structuring remains unclear. This study investigated whether an antibiotic and an anesthetic contribute to network formation during membrane fabrication. Membranes were prepared by solvent casting from molded bicomponent hydrophilic biopolymer hydrogels, using calcium gluconate as a reference ionic crosslinker. The hydrogel-to-membrane transition was monitored by single-sided ^{1}H NMR at 34 and 40 °C through drying profiles and T_1/T_2 relaxation measurements. Complementary ^{23}Na benchtop NMR experiments were performed to investigate formulation-dependent changes in the ionic environment. Drying profiles showed matrix contraction followed by dimensional stabilization despite continued evaporation. Crosslinked formulations exhibited two drying regimes independent of temperature, whereas non-structured systems showed one. The transition to the slower regime occurred at a membrane thickness of ~1.1 mm regardless of temperature, suggesting that membrane formation and surface barrier development are driven by structural rather than thermal effects. All formulations reached a similar final thickness, independent of crosslinker and temperature, although faster at 40 °C than at 34 °C. Membranes containing APIs showed restricted molecular mobility comparable to calcium-gluconate-crosslinked systems. Preliminary ^{23}Na NMR results indicated formulation-dependent ionic interactions during network formation. These findings indicate that APIs actively contribute to network development during membrane formation. The resulting structural constraints are comparable to those achieved with a conventional ionic crosslinker, supporting the design of self-structuring drug-loaded biopolymeric membranes without additional crosslinking agents.

Acknowledgements
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Facility-scale NMR studies of complex mining tailing materials

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Mining tailings storage facilities (TSFs) require reliable methods for assessing sedimentation, compaction, and drying, since these processes directly affect water recovery, geotechnical stability, and long-term environmental performance. In our recent work, we established a portable single-sided NMR methodology based on the NMR-MOUSE for monitoring water-content and water-mobility changes in complex gold-mine tailings through ^{1}H signal amplitudes and transverse relaxation times (T_2). The method was validated against tailings samples from a TSF in Lapland, Finland, and revealed clear relationships between NMR response, particle-size distribution, mineral composition, solids content, and the kinetics of sedimentation and dewatering.

In this contribution, we extend that methodology from controlled laboratory studies toward facility-scale assessment of beach-deposited tailings in Lapland. Measurements collected from different locations and depths are used to evaluate spatial variability in tailings behavior across the deposit and to test how well the NMR observables reflect local differences in consolidation state and moisture distribution under field-relevant conditions. Emphasis is placed on the capability of the method to distinguish rapid short-term settling from slower structural reorganization and drying, and to identify zones where mineralogical and granulometric heterogeneity control the NMR response. The approach follows the framework established in our recent publication, where faster-settling samples were associated with coarser particles and higher final T_2 values, whereas finer and more heterogeneous materials showed delayed settling and more restricted water mobility.

The results demonstrate that portable single-sided NMR has strong potential for near-real-time characterization of tailings at the facility scale. By linking NMR measurements with physical and mineralogical properties, the method support sustainable tailings management.

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Probing Solid-Liquid Separation Dynamics in Anaerobic Digestate via 1D and 2D Low-Field NMR Relaxometry

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Anaerobic digestate (AD) is a nutrient-rich residue of anaerobic digestion with potential as a biobased fertiliser, yet conventional metrics like turbidity and total solids are time-intensive and lack structural sensitivity. LF-NMR relaxometry offers a non-invasive route to characterise water distribution independently of sample opacity. Treating flocculated digestate as a porous medium with free (P1), interstitial (P2), and vicinal (P3) populations, this work applies 1D and 2D LF-NMR to two AD feedstocks. Red meat (RM) AD and food water (FW) AD were conditioned with flocculant (EM640CT (0.41% active)) across 0 to 4.5 and 0 to 25.5 wt%, and monitored using a 12.7 MHz Oxford GeoSpec and 14 MHz ilumr. T_2 CPMG (25,000 echoes, t_e = 300 µs), T_1-T_2 IR-CPMG[4] (32 steps, 10,000 echoes), and T_2-T_2 CPMG-CPMG (t_e = 300 µs, t_{mix} = 5 to 300 ms) were applied; T_2 resolved by regularised inversion into four populations (P1 to P4). For RM-AD, polymer conditioning produced a T_2 shift from 0.19 to 1.77 s, transitioning the dominant population from interstitial (P2) to free water (P1) beyond a critical threshold, a nearly fivefold increase in recovered solids. For FW-AD, the same flocculant at doses up to fivefold higher produced negligible T_2 redistribution, consistent with EPS, DOM, and FOG-driven inhibition. T_1-T_2 maps confirmed T_1/T_2 proportionality with surface-to-volume ratio. T_2-T_2 exchange spectroscopy revealed off-diagonal cross-peaks (P2-P3) at t_{mix} = 100 ms in RM-AD, a coherence length ~35 µm; no exchange peaks detected in FW-AD. 1D and 2D LF-NMR resolve microstructural changes inaccessible to conventional process metrics. T_2-T_2 exchange reveals the same polymer produces a coherent ~35 µm network in RM-AD but fails in FW-AD, undetectable by turbidity or total solids metrics. Future work will integrate mobile LF-NMR into a pilot-plant AD facility for continuous flocculation monitoring.

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Single-Sided NMR Relaxometry and Diffusometry Across Porous Media Applications

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Single sided NMR provides a framework for performing portable, non-invasive investigations of porous media through depth-selective relaxometry and diffusometry. The NMR-MOUSE device was exploited with 1D profiling and multidimensional correlation experiments to extract quantitative markers of layer structure, pore connectivity, and fluid transport in heterogeneous porous systems spanning cultural heritage[1,2], cementitious materials, and biological tissues[3]. In the case of paintings on canvas[1], T_2 distributions and signal-intensity depth profiles are correlated with stratigraphic cross-sections. This approach enhances the identification of textile support, preparatory grounds, and paint layers. Furthermore, it highlights the challenges intrinsic to inhomogeneous, partially overlapping strata that contribute jointly to the sensitive volume. About stone conservation[2], single-sided profiles are used to evaluate penetration depth and homogeneity of consolidation treatments. In cement pastes, low-field measurements have been shown to monitor hydration-driven decreases in T_1 and T_2. Furthermore, via T_1–T_2 correlation maps, these measurements have been demonstrated to resolve interlayer and gel-pore water populations, characterised by distinct T_1/T_2 ratios and sensitivity to binder composition and paramagnetic iron content. In the field of biomedical studies, the exploitation of strong static gradients for diffusion-weighted contrast is a key approach. Diffusion-weighted T_1–T_2 encoding has been shown to suppress muscle/cartilage signal, thereby enabling trabecular-bone BV/TV estimation. Furthermore, depth-wise multiparametric mapping of articular cartilage[3], supported by multivariate data analysis, provides a method of differentiating layered structures. Collectively, these studies demonstrate the effectiveness of single-sided NMR as a powerful and versatile tool for in situ diagnostics, monitoring of treatments and microstructural evolution in a wide range of porous media.

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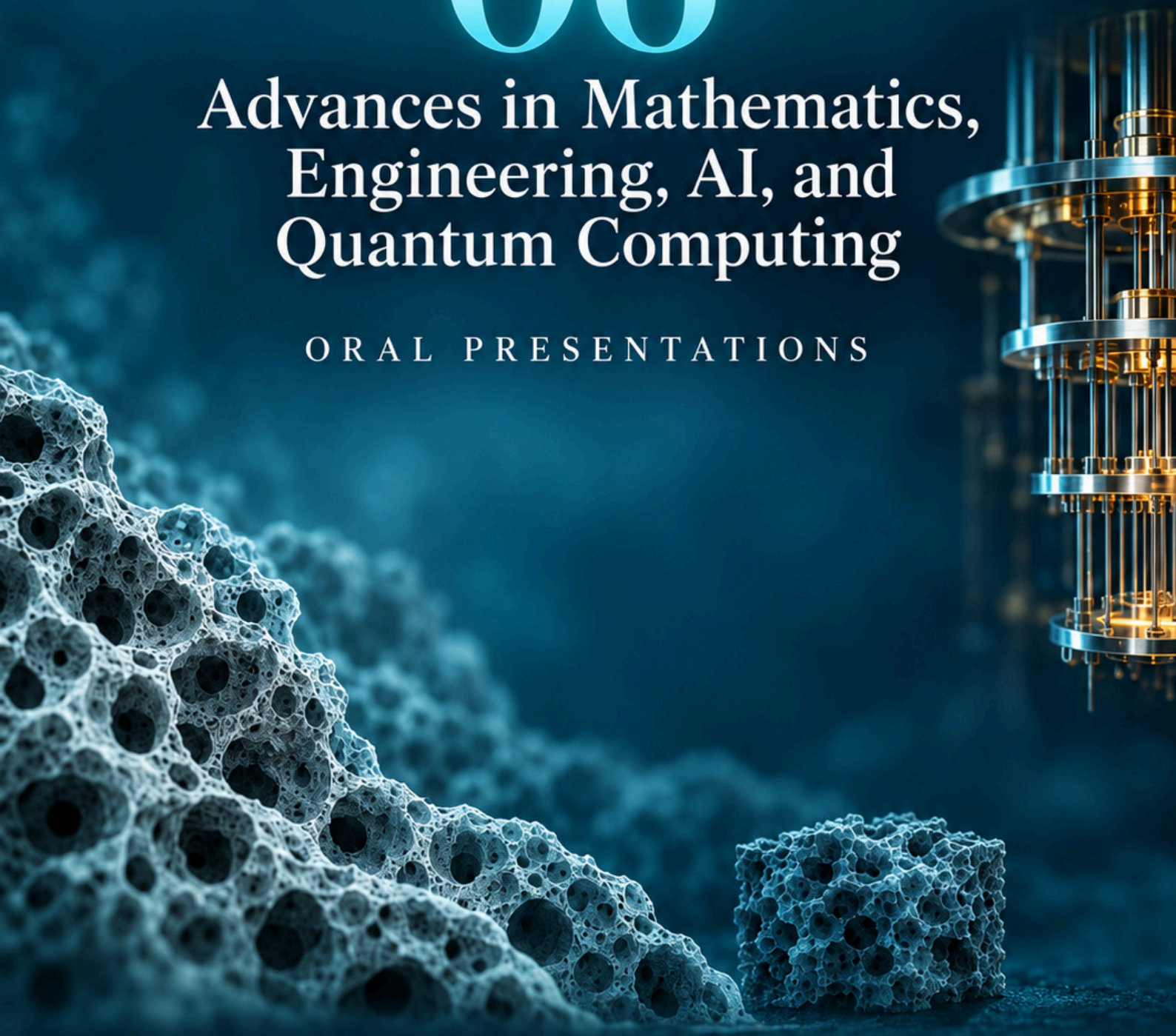
17th International Bologna Conference on Magnetic Resonance in Porous Media

SECTION

06

Advances in Mathematics, Engineering, AI, and Quantum Computing

ORAL PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

OCTOBER 26–30, 2026

A compative study of effective surface relaxation estimation using two NMR relaxometry inverse modeling approaches

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This talk presents a comparative analysis of two advanced inverse modeling approaches for estimating the properties of porous media from NMR relaxometry signals. While inverse NMR relaxometry (T_1/T_2 distribution recovery) is a fundamental technique for characterizing pore-scale structures based on surface-influenced molecular relaxation, the choice of inversion methodology has a critical impact on the reliability and efficiency of the results. We specifically evaluate a rigorous **Bayesian framework with Markov Chain Monte Carlo sampling (MCMC)** [1] against a modern **Physics-Informed Neural Network (G-PINN) based on a Galerkin formulation** [2]. The comparison is made in terms of numerical accuracy, uncertainty quantification, and computational performance. Using synthetic NMR relaxometry signals—generated from both analytical and direct numerical models—the two approaches for estimating the **effective surface relaxation** are compared. The details of the complete methodological process are presented, encompassing mathematical formulations, numerical discretizations, and computational implementations, providing a guide for selecting an inversion approach tailored to the quality of the data and the specific requirements of the application.

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Constante, L., Pires, A., Díaz-Viera, M.A. (2026). Galerkin Physics-Informed Neural Network Approach for Inverse Problems. Application to Estimation of Tracer Dispersion in Porous Media, Computational Geosciences 30(24).

A Two-Stage Galerkin Physics-Informed Neural Network Approach for Forward and Inverse Nuclear Magnetic Resonance Modeling at the Pore Scale

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Nuclear Magnetic Resonance (NMR) is widely used in reservoir characterization to evaluate pore-scale properties and fluid behavior in porous media. However, solving forward and inverse pore-scale NMR problems remains computationally challenging due to the coupled diffusion-relaxation mechanisms governing magnetization dynamics. Conventional numerical methods often require fine spatial discretization and high computational cost, particularly in inverse workflows. This work proposes a Pre-Trained Galerkin Physics-Informed Neural Network (pG-PINN) (Constante *et al.*, 2026) approach for solving direct and inverse pore-scale NMR problems in spherical pores. The methodology combines Galerkin-based domain decomposition with physics-informed learning to approximate the Bloch–Torrey diffusion-relaxation equation under diffusion-controlled relaxation conditions. Multiple compact neural subnetworks act as adaptive basis functions, improving training stability and solution accuracy near pore boundaries, where relaxation effects dominate. For the forward problem, the model predicts the spatiotemporal evolution of magnetization and reconstructs NMR relaxation responses for different pore radius, diffusion coefficients, and surface relaxivities. For the inverse problem, the pG-PINN estimates surface relaxivity directly from synthetic NMR relaxation responses. A two-stage pre-training strategy is introduced to accelerate convergence and improve parameter identification. The proposed approach was validated against analytical solutions for spherical pore geometries. Results demonstrate that the pG-PINN achieves high accuracy with reduced computational cost compared with conventional numerical approaches while maintaining robust inverse estimation capability under noisy conditions. The methodology provides an efficient and flexible alternative for AI-driven pore-scale NMR modeling and digital rock physics applications.

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Categorical Diversity Optimization: A framework for inversion and component analysis of NMR data

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Classification of probed nuclei in NMR relaxometry via relaxation rate spectra is presented as a paradigmatic Categorical Inverse Problem (CIP)—a mixture model problem aiming to find a distribution of known types proportionally linked to a dataset. Here, the categorical set is a partitioned interval, mapping relaxation rate bands onto signal amplitudes via a discretized continuous response model related to the Laplace transform.

I define CIP generally to emphasize its normalization condition and present proper data preconditioning and denoising strategies for applying the principle of Categorical Diversity Optimization: Selection of either the most or least diverse distributions representing a solution set.

By varying diversity measures, the framework establishes a continuum of well-posed inverse problems for any dataset, proving a continuum of uniquely characterized distributions exists as special CIP solutions. This quality unifies traditional inversion methods like Entropy Maximization, Non-negative Least Squares, and the Minimax Principle under a single banner.
Effective 1D and 2D computational algorithms to compute these solutions are advanced, alongside theoretical results on their categorical support and the influence of noise.

As diversity measures differ mainly on how they weigh the contribution of rarer categories, their choice yields distinct qualitative and quantitative descriptions, yet numerical maximal diversity solutions display a remarkable consistency of signatures. Comparisons of minimal and maximal diversity solutions for polyexponential signal decay exemplify the impact of optimization principle.

Finally, the framework's versatility is demonstrated by unmixing problems based on NMR relaxometric data, where mixed signals of unknown proportions are decomposed using a few referential component decays. Potential applications in Quality Control and Petrophysical Evaluation are considered together with current methodological limitations.

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Mapping local foam mobility in porous media from computed tomography data

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Recovering apparent viscosity and foam texture fields from coreflooding experiments is challenging, even with modern computed tomography (CT) scan equipment. In this work, we present an explicit expression for efficiently calculating the effective foam viscosity and propose an improved procedure for processing CT scan images to obtain accurate water-saturation profiles. Using these techniques, we processed CT scan data from a coreflooding experiment, showing that the increase in effective foam viscosity due to foam generation occurs early during injection, before breakthrough. The rapid increase in apparent viscosity is due to foam formation before breakthrough. After the breakthrough, the foam texture reaches its maximum, and the effective foam viscosity increases logarithmically over time as the foamed gas sweeps out the water phase. The pressure drop obtained using the effective foam viscosity showed good agreement with the experimental values before breakthrough. The workflow proposed here could be readily adapted to other foam models, provided reasonable estimates for these new quantities can be determined from experiments.

Acknowledgements
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Microfluidics as a Tool to Study Pore-Scale Phenomena in Complex Multiphase Flow in Porous Media

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Multiphase flow in subsurface formations is ubiquitous in both oil production and CO2 storage. The non-linear nature of the flow leads to complex fluid displacement mechanisms that operate across various scales, from pore-level to Darcy scale. Accurate flow models, necessary in the design and optimization of injection processes, require detailed description of pore scale multiphase flow. Traditionally, flow behavior at different temperature and pressure conditions is evaluated on laboratory-scale experiments using core-flooding systems, PVT cells and other equipment. The experiments are expensive, require long measurement times and large volumes of fluids. In this context, microfluidics emerges as a valuable technique. Improvement on the fabrication of microfluidic devices and flow control have led to growth in the use of microfluidics to gain fundamental understanding of pore-scale multiphase flow, enabling the correlation between pore scale events and macroscopic flow characteristics, and phase behavior. Recent developments allow microfluidic experiments to be run at high pressure and high temperature conditions, allowing the determination of minimum miscibility pressure between CO2 and crude oil in approximately 30 minutes and using only 0.1 mL of oil sample for each data point.

Here, we report various multiphase flow analyses using porous media microfluidic devices to examine oil displacement by water, emulsions, and foam, as well as CO2 storage in saline aquifers. By visualizing pore-scale phenomena, we can correlate these events with macroscopic flow characteristics, which may be leveraged to optimize subsurface processes.

Acknowledgements

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Quantum Computing and Porous Media: Applications in CO2 Capture & Storage

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Mitigating climate change requires efficient computational frameworks for simulating CO2 capture and storage. In this presentation, I introduce an open simulation environment for pore-scale assessment in digital rock [1] that creates accurate capillary network representations [2] based on microscopic tomography data taken from sandstone and carbonate rock plugs [3]. Single-phase and two-phase flow simulations within a digital rock's capillary network can be performed assuming realistic reservoir conditions. One research use case of the simulator is the injection of super-critical carbon dioxide into sandstone, for optimizing carbon dioxide saturation as function of temperature and pressure, respectively [4]. For predicting the long-term geologic storage of carbon dioxide, the simulator tracks computationally the modifications caused by carbon mineralization within each capillary of the connected pore space [1]. The process gradually reduces the diameter of capillaries over time and causes the porosity and permeability of the rock to degrade. If flow conditions are not optimized, a rock might not achieve its full geologic storage potential.

While having the potential for improving the simulation of flow in digital rock, current applications of quantum computing are mainly in the prediction of materials properties at molecular scale [5]. One example is the binding of carbon dioxide in nano-pores designed for application in direct air capture [6]. Hybrid, quantum-classical algorithms on pre-fault tolerant quantum processing units deliver useful predictions and are a promising approach for advancing the discovery of novel materials for carbon dioxide capture.

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Quantum Computing Applied to Oil & Gas Problems

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The oil and gas exploration industry demands the use of high-performance computing for subsurface modeling from seismic data. Such modeling supports decision-making regarding the drilling of new wells, a decision that involves investments on the order of hundreds of millions of dollars. Quantum computing emerges in this context as a promising tool, proposing algorithms capable of accelerating the solution of numerical problems, notably the so-called inversion problem. Other relevant applications that have been explored by quantum computing include, significantly, simulations of wave propagation in heterogeneous media and the search for new materials with potential for carbon capture. On this talk, these applications will be discussed, as well as the main bottlenecks of quantum computing regarding industrial applications.

Acknowledgements
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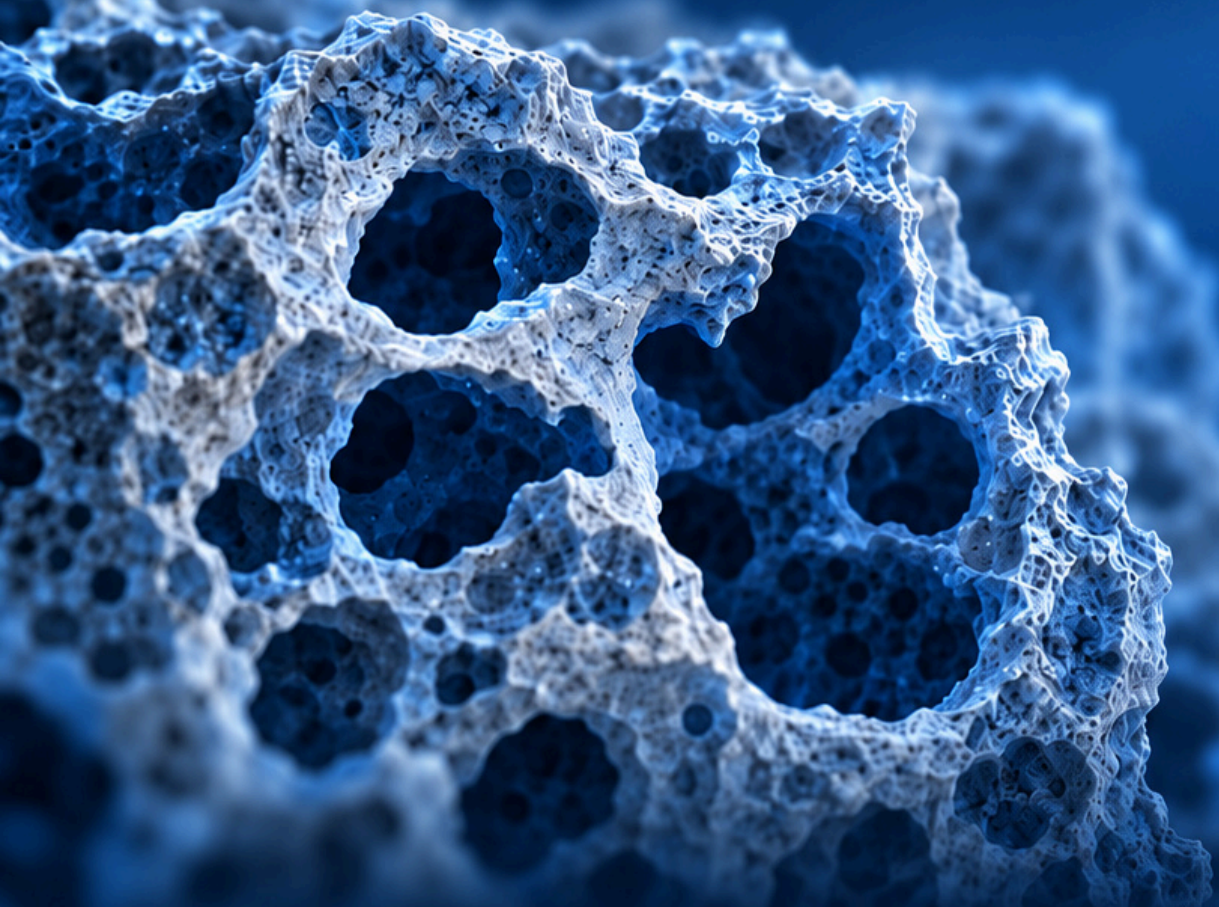
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Magnetic Resonance in Porous Media

SECTION

01

Digital Porous Media & NMR

POSTER PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

OCTOBER 26–30, 2026

Bayesian framework for inverse modeling in estimating porous media properties from Nuclear Magnetic Resonance signals

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Quantitative analysis of Nuclear Magnetic Resonance (NMR) relaxation data is essential for characterizing heterogeneous porous media. Outside the fast-diffusion regime, traditional inversion methods that assume a mono-exponential decay per pore oversimplify the problem, leading to a severely ill-posed inverse problem where surface relaxivity and pore size cannot be independently resolved without multi-modal or regularized approaches (Morales-Chávez et al., 2025).

To overcome this challenge, this work proposes a robust probabilistic inverse modeling framework based on a non-dimensional formulation of the Bloch-Torrey equation. Building upon recent advancements in probabilistic modeling for NMR parameter extraction (Li et al., 2021), the forward problem is solved with the Finite Element Method (FEM) and rigorously validated against the semi-analytical Brownstein-Tarr solution. Bayesian inference is performed via the t-walk Markov Chain Monte Carlo algorithm (Christen et al., 2010) to estimate the dimensionless surface relaxivity (α) and pore radius (φ_R) and then verified through twin experiments using synthetic data with additive Gaussian noise.

A comprehensive set of eight test cases were evaluated, systematically varying physical parameters across the fast, intermediate, and slow diffusion regimes, with pore radii ranging from 1 μm to 1000 μm and surface relaxivities from 3 μm/s to 40 μm/s. Results demonstrate that the non-dimensional formulation effectively decorrelates the parameters, thereby resolving the degeneracy. Maximum A Posteriori (MAP) estimates recover the true petrophysical properties with high accuracy and robustness, accompanied by rigorous uncertainty quantification.

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Computational toolkit for simulating the Nuclear Magnetic Resonance response of porous media

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Here we introduce an in-house developed computational toolkit for simulating the Nuclear Magnetic Resonance response of porous media. The collection of Python implementations uses high-performance parallelism strategies to simulate Nuclear Magnetic Resonance experiments from 3D microtomographic digital images. Our toolkit has been employed to investigate direct and inverse problems considering different applications, including relaxometry, diffusiometry, multi-tau, and DDIF. Among the investigations, we may emphasize advanced strategies to estimate the surface relaxivity, statistical analysis and uncertainty propagation in relaxometry, and the feasibility of using machine learning for permeability estimations. Further, our implementations served as basis for the development of a virtual Nuclear Magnetic Resonance profiling tool.

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Pore size distribution from NMR and image based methods: A comparative studyBENAVIDES, F.; et al. Pore size distribution from NMR and image based methods: A comparative study. Journal of Petroleum Science and Engineering, v. 179, p. 829–839, 2019. DOI: 10.1016/j.petrol.2019.04.083.

Evaluating Magnetic Surface Relaxivity through NMR Simulations in Digital Porous Media

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The fourth-generation synchrotrons deliver low- to high-energy X-rays with high photon flux, enabling high-resolution 3D tomography within seconds when combined with advanced detectors. The MOGNO beamline [1] at the Brazilian Synchrotron Light Laboratory (LNLS), located at Brazilian Center for Research in Energy and Materials (CNPEM), provides nano- to micrometer-scale computed tomography for multiscale analysis, including zoom tomography with a spatial resolution of approximately 200 nm and 4D imaging through *in situ* experiments with time resolutions on the order of a few seconds. Within this context, current efforts focus on integrating microtomography with complementary techniques to elucidate the physicochemical behavior of porous materials, particularly fluid–solid interactions and transport processes at the pore scale. Nuclear Magnetic Resonance (NMR) plays a central role in porous media characterization, both in laboratory studies and *in situ* applications. NMR enables fluid characterization while also providing morphological information, such as pore-size distribution and pore connectivity. Furthermore, wettability and magnetic surface relaxivity, parameters governed by the rock mineralogy, influence relaxation times and provide additional insight into the properties of porous media [2].

The integration of zoom tomography with NMR therefore offers a promising framework for investigating porous media under both static and dynamic conditions. In this work, we present NMR simulations in digital porous media and compare the magnetic surface relaxivity estimated directly from NMR measurements with that obtained from computational simulations.

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Exploring the preasymptotic regime in synthetic rocks coated by goethite

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Nuclear magnetic resonance has been an essential tool for non-invasive investigations of complex porous media and the extraction of relevant petrophysical parameters from relaxation rates obtained in signal decay experiments such as CPMG. In the free regime, the relaxation rates contain geometric (Brownstein–Tarr)[1] and diffusion (Torrey)[2] contributions, leading to a linear dependence with squared echo time (t_E). However, for long t_E values and/or high magnetic mineral content, the diffusion contribution is no longer described by the Torrey term and the experimental data become nonlinear. In this case, the spin ensemble gradually evolves to asymptotic regimes known as motional averaging or localization. Before reaching the asymptotic regime, a preasymptotic behavior emerges, producing a nonlinear monotonic increase of the relaxation rates that remains poorly explored. In this work, the preasymptotic regime was investigated in sintered porous rocks by varying t_E (100–600 μs) and increasing the goethite content (0–128 ppm). For short t_E, the relaxation rates exhibited a linear dependence with squared echo times at low concentrations. Increasing the goethite content progressively reduced the linear range, indicating suppression of the free regime. The nonlinear data were fitted using a recent model that replaces the Torrey diffusion term with a logarithmic dependence on echo time[3]. From this model, the critical time associated with the transition to the asymptotic regime was extracted, showing a reduction of about 67 % at the highest goethite concentration. The characteristic lengths of the asymptotic regimes were also evaluated. The results indicate that localization dominates the asymptotic regime, suggesting that spins mainly lose phase coherence due to the enhanced internal gradient field generated by the magnetic minerals, estimated as ≈ 4.0 T/m. These findings provide insights into the nonlinear behavior of relaxation rates.

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Permeability Estimation in Heterogeneous Pre-Salt Carbonates: A Multicomponent Model Based on NMR T2 Distributions from Well Logs

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Permeability estimation in carbonate reservoirs represents a significant challenge due to their high heterogeneity. In these systems, the complexity of the pore structure, characterized by different pore-size distributions, varying degrees of connectivity, and a strong influence of depositional and diagenetic processes, often results in a non-linear porosity–permeability relationship. In this context, this study evaluates the application of a multicomponent permeability model based on transverse relaxation time (T2) distributions obtained from nuclear magnetic resonance (NMR) well logs. The proposed approach aims to classify the pore system into distinct groups, considering the contribution of different pore populations in order to improve permeability prediction. The study area corresponds to the Atapu Field, located in the Santos Basin, Brazil, within the geological context of the Pre-Salt. Its carbonate reservoirs exhibit pronounced heterogeneity, with the occurrence of interparticle, vuggy, and moldic porosity, associated with dissolution and fracturing processes, which directly affect fluid flow. The permeability estimates obtained from the multicomponent model were compared with those derived from conventional SDR and Timur–Coates (TC) models. The results showed that the multicomponent approach provided more accurate and reliable permeability estimates, thereby improving the ability of the parameter to reflect pore connectivity and pore-size distribution with greater precision. Therefore, the proposed methodology contributes to a more detailed and accurate petrophysical characterization of Brazilian Pre-Salt carbonate reservoirs.

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Spectral parameters of the T_2 distribution for heterogeneity characterization and permeability estimation in carbonates by NMR

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Estimating permeability in heterogeneous carbonates from NMR data remains challenging because the classical SDR and Timur-Coates models rely solely on T_{2LM} and FFI/BVI as proxies for pore structure, overlooking the full pore-size distribution. This work proposes the sorting of the T_2 distribution, defined as the amplitude-weighted standard deviation in $\log_{10}(T_2)$, as an auxiliary permeability predictor, combined with NMR porosity (Φ_{NMR}), in a set of 10 carbonate samples from Morro do Chaves Formation, Sergipe-Alagoas Basin. Gaussian decomposition of the T_2 curves showed that 8 samples are trimodal and 2 are bimodal, with pore populations spanning micropores (T_2 < 30 ms), meso/macropores, and supramacropores (T_2> 200 ms). Among the heterogeneity indices computed (skewness, kurtosis, Shannon entropy, sorting, and coefficient of variation (CV)), sorting ($r = -0.74$, $p < 0.05$) and CV ($r = -0.76$, $p < 0.05$) showed the strongest correlation with log(k) and distinguished the more permeable samples more effectively than the scalar parameters T_{2LM} and FFI/BVI. The partial correlation of sorting controlling for Φ_{NMR} reached $r = -0.85$ ($p = 0.002$), confirming that the spread of the T_2 distribution carries permeability-relevant information independently of pore volume. The parsimonious model ($k = 11.08 \cdot \Phi^{2.42} \cdot 10^{-1.26\mathrm{slog}(T2)}$), calibrated by log-log regression and validated by leave-one-out cross-validation (LOO-CV) with 2000-resample bootstrap, achieved R^2 LOO = 0.595 and RMSE LOO = 0.223, outperforming SDR (R^2 LOO = 0.550), Han's model (0.376), and Timur-Coates (0.327). Four-parameter models (Φ + sorting + T_{2LM} or CV) degraded LOO performance, confirming that sorting complements porosity without requiring additional predictors for this dataset. Taken together, these results suggest that the shape of the T_2 distribution carries structural petrophysical information that remains underexplored in conventional NMR permeability models for carbonates.

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Water mobility during gypsum hydration and drying: Relationships with hydration kinetics and mechanical strength assessed by low-field NMR

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Gypsum plaster strength is strongly affected by water retained after hydration, making it important to distinguish chemical reactions from subsequent drying. This study investigated water mobility during calcium sulfate hemihydrate hydration and assessed the relationship between NMR indicators and compressive strength. Plasters with water-to-gypsum ratios of 0.50, 0.55, and 0.60 were characterized by low-field ^{1}H-NMR using CPMG. Transverse relaxation (T_2) distributions were monitored during the first hour, and signal intensities were evaluated up to 7 days under sealed and oven-dried conditions. Isothermal calorimetry, thermogravimetry, and compression tests complemented the analysis. During early hydration, the dominant, longer-T_2 peak decreased in intensity, while a secondary, shorter-T_2 population shifted toward longer relaxation times, suggesting changes in water mobility and the developing crystalline microstructure. The evolution of the CPMG signal was associated with cumulative heat release, linking changes in detectable water to hydration kinetics. Under sealed conditions, NMR intensity decreased initially and remained nearly stable from 1 to 7 days. In oven-dried specimens, the signal declined further, consistent with moisture removal. The NMR-derived indicator for dried specimens correlated more strongly with compressive strength (R^2 = 0.938) than the indicator for sealed specimens (R^2 = 0.467), and showed a correlation comparable to thermogravimetry (R^2 = 0.958). These findings indicate that low-field NMR can distinguish hydration-related water redistribution from drying effects relevant to gypsum mechanical performance.

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Magnetic Resonance in Porous Media 2026

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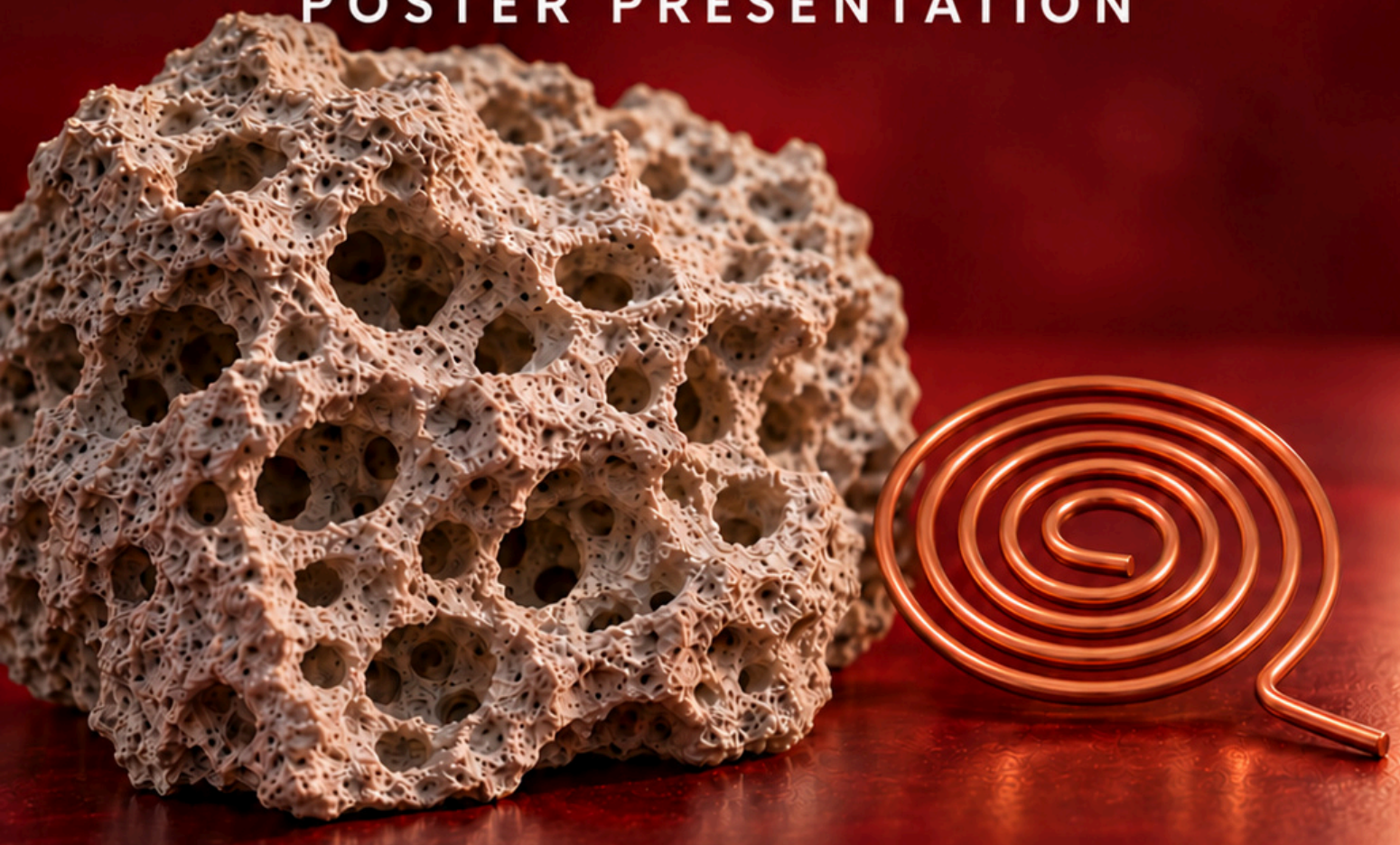
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SECTION

02

NMR Methods & Instrumentation

POSTER PRESENTATION



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

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Bicontinuous Microemulsions as Dynamic Nanostructured Media: Composition-Dependent Molecular Dynamics Probed by FFC-NMR Relaxometry

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Bicontinuous microemulsions are macroscopically homogeneous and isotropic systems, yet their nanoscale organization can give rise to complex molecular dynamics [1]. In these systems, oil-rich and water-rich domains form interconnected pathways organized around a surfactant-rich interfacial region, creating a dynamic nanostructured medium in which molecular motions occurring over different length and time scales may coexist. Understanding how composition modulates these motions is essential for linking internal organization to transport and relaxation behavior in complex soft media. Here, fast field-cycling nuclear magnetic resonance (FFC-NMR) relaxometry was used to selectively probe the composition-dependent dynamics of the surfactant Tergitol 15-S-9 in bicontinuous microemulsions. Because the oil and water phases were deuterated, the measured proton relaxation dispersion predominantly reflects the motion of the surfactant within the interfacial environment. Three formulations were compared to represent distinct compositional regimes: ME1, a water-rich system; ME2, an oil-rich system; and ME3, a surfactant-rich system. The resulting proton relaxation dispersion profiles revealed marked differences among the samples, indicating that variations in oil, water, and surfactant content strongly influence surfactant mobility within the bicontinuous microstructure. Differences among the ME1, ME2, and ME3 relaxation dispersion profiles are consistent with changes in hydration, oil swelling, surfactant packing, and interfacial organization, showing that samples classified within the same broad bicontinuous region exhibit distinct dynamic signatures. These results highlight FFC-NMR relaxometry as a sensitive approach for probing surfactant dynamics in soft nanostructured media, providing insight into the coupling between internal organization and molecular motion in bicontinuous microemulsions.

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Development of a Rheo-NMR instrument to study dynamical material properties

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Instrumentation combining rheological and NMR measurements was first introduced in the literature three decades ago[1]. Nevertheless, adoption to this day is limited, and no commercial options exist in the market. With such techniques, the molecular properties probed by conventional NMR methods can be studied under precisely controlled deformation, while simultaneously measuring macroscopic rheological properties of materials (shear/extensional).

Materials incorporating weak bonds (either covalent or supramolecular) in their molecular structure have attracted attention due to their useful mechanical properties[2]. Under deformations, these weak bonds would break before the stronger chemical bonds of the molecule and subsequently re-attach, returning to their equilibrium positions once the deformation ceases. Such behaviour can introduce useful features into materials, such as self-healing and improved toughness. However, these properties have so far been difficult to quantitatively assess at the molecular level in-situ during deformation.

Our project aims to develop experimental methods combining rheology and time-domain NMR to investigate polymer samples involving weak bond structures. We develop an in-house Rheo-NMR setup based on a commercial rheometer, a low-field (0.3T) pseudo-Halbach magnet[3] and a radio-frequency probe, enabling such measurements on the bench top. We will present the operational principles of this device, preliminary measurements, and challenges.

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Dipolar-Filtered Magic Sandwich Echo: A Self-Normalized Approach for NMR Cryoporometry of Mesoporous Materials

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NMR cryoporometry is a well-established technique for determining pore size distributions by monitoring the melting behavior of confined fluids in porous materials. Conventional methods rely on spin-echo experiments and external reference measurements to compensate for temperature-dependent signal variations. An alternative approach based on the Dipolar-Filtered Magic Sandwich Echo (DFMSE) pulse sequence is presented.

The proposed method combines acquisitions performed with short and long dipolar filter times, providing an internally normalized signal that eliminates the need for external references while compensating for Curie-law effects and instrumental variations. Furthermore, the filter-time dependence offers a simple criterion for suppressing non-cryoporometric contributions, improving the accuracy of pore size determination.

The methodology was validated using porous silica and controlled-pore glass samples saturated with water and cyclohexane. The resulting pore sizes and pore size distributions showed excellent agreement with conventional NMR cryoporometry and nitrogen adsorption measurements. The approach was also successfully applied to a cadmium imidazolate metal-organic framework, demonstrating its applicability to structurally complex porous systems.

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Direct Determination of Pore Size Distribution from Multi-Temperature MR Relaxation Measurements

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Brownstein-Tarr (BT) theory provides a comprehensive framework for understanding magnetic resonance (MR) relaxation in porous media. In our previous work, BT theory was validated experimentally and shown to explain the temperature-dependent MR relaxation behaviors observed in a wide range of porous materials [1-3]. In this presentation, we further extend the theory by introducing direct methods for determining pore size distribution and surface relaxivity from MR relaxation measurements.

The MR T_2 distribution is widely used as a proxy for the pore size distribution. However, this relationship is generally valid only in the fast-exchange BT regime and requires independent calibration of the surface relaxivity. These requirements limit the practical application of MR pore size characterization. Our recent work overcomes these limitations by exploiting the temperature dependence of T_2 relaxation in paramagnetic sandstones, when relaxation occurs in the intermediate BT regime. The determined surface relaxivity enables quantitative conversion of T_2 distributions into pore size distributions. The BT number of 0.1, marking the boundary between the fast-exchange and intermediate BT regimes, is found to lie close to the conventional T_2 cut-off value, providing a physical explanation for this empirical criterion.

We will also present a direct inversion method for determining pore size distributions directly from multi-temperature CPMG decays. Multi-temperature measurements generate temperature-dependent relaxation kernels through the fluid diffusivity. The pore size distribution and surface relaxivity are determined simultaneously by inversion of the multi-temperature CPMG decays. The method is validated using both simulation and experimental data from glass bead packs and porous rocks. The recovered pore size distributions show excellent agreement with imaging methods, demonstrating the robustness and broad applicability of the proposed method.

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Effects of Temperature-Dependent Surface Relaxivity on Variable-Temperature NMR Pore Size Measurements

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In this work, we build upon the method developed by Balcom and co-workers, who proposed a direct approach for measuring pore size and surface relaxivity using variable-temperature magnetic resonance experiments [1]. Their method estimates pore size and surface relaxivity by exploiting the relationship between the transverse relaxation time (T_2) and the temperature dependence of the self-diffusion coefficient of the saturating fluid. It combines variable-temperature Carr-Purcell-Meiboom-Gill (CPMG) measurements with nonlinear fitting based on three idealized pore geometries: planar, cylindrical, and spherical. In the original approach, the temperature dependence of the water self-diffusion coefficient was taken from literature data [2], while the surface relaxivity was assumed to remain constant over the investigated temperature range. In the present work, we investigate the limits of validity of the constant surface-relaxivity assumption by comparing the original model with an alternative approach in which the surface relaxivity is allowed to vary with temperature according to functions reported in the literature [3]. Numerical calculations were performed to determine the range over which the constant-relaxivity approximation remains valid and to identify signatures that can be used to establish its limits of applicability. The proposed criteria were then used to analyze experimental data obtained from glass-bead samples with nominal pore sizes of 36 and 112 μm and from a silica gel sample with pore sizes ranging from 30 to 70 μm. In all cases, the estimated pore sizes were in good agreement with the expected values. Applications to rock core samples and porous biomasses are currently under investigation.

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Electromagnetic Design and Optimization of a Quadrature RF Probe for Single-Sided NMR at 13 MHz

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Single-sided nuclear magnetic resonance (NMR) enables non-invasive characterization of materials and porous media without the geometrical restrictions of conventional closed-bore magnets. Systems such as the NMR-MOUSE allow relaxation and diffusion measurements in highly inhomogeneous magnetic fields and have been applied to moisture and porous-material characterization [1]. Quadrature RF probes can further improve NMR performance by reducing the RF power required to generate a given transmit field by a factor of two and increasing receive signal-to-noise ratio (SNR) by a factor of √2 compared with linear polarization [2]. This work investigates, through electromagnetic simulations, a quadrature RF probe operating at 13 MHz for a PM10 NMR-MOUSE system. The proposed configuration combines a D-shaped coil and a planar spiral coil to generate approximately orthogonal RF magnetic-field components. Simulations were performed in COMSOL Multiphysics at 13 MHz, with the spiral coil positioned 5 mm above the D-shaped coil and both ports excited with equal amplitudes and a 90° phase difference. Matching and tuning networks were optimized for 50 Ω. The selected D-shaped coil had a 40-mm radius, two loops, and a simulated inductance of 1064.27 nH, with optimized matching and tuning capacitances of 10.7 pF and 132.0 pF, respectively. Spiral coils with radii from 15 to 36.8 mm and five or seven turns were evaluated. Quadrature performance was assessed from the circularly polarized RF field components [2], identifying six configurations with satisfactory behavior. These preliminary results demonstrate the feasibility of quadrature RF excitation in a single-sided NMR sensor and provide a promising approach to improve RF efficiency and sensitivity while reducing transmit power requirements for NMR studies of porous and heterogeneous materials.

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FFC-NMR STUDY OF WATER-PROTEIN DYNAMICS IN DAIRY PRODUCTS WITH AN INVERSION-DEDICATED TOOL

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Nowadays, Fast Field Cycling (FFC) NMR is gaining recognition as a powerful technique to probe the molecular dynamics (MD) of various materials, including applications in material science, biomedical, environmental sectors, and food[1].

By varying the magnetic field strength and thus the Larmor frequency, it is possible to probe MD over a wide range of timescales from fractions of nano- to micro-seconds. The acquired data are usually displayed in the form of a nuclear magnetic resonance dispersion (NMRD) profile, $R_1 = 1/T_1$ versus the Larmor frequency.

Despite FFC-NMR being a powerful technique, interpreting NMRD profiles to understand the MD that characterize them is not straightforward; complex models (conceptual models) are required to describe the various processes (interactions) that can occur in the sample. In principle, the expression for R_1 is related to the Fourier transform of the appropriate correlation function, which takes into account all the phenomena and processes that occur through characteristic parameters (correlation times).

Here we present a MATLAB-based inversion tool expressly designed for the Bryant and Korb (BK) model for hydrated proteins, which is used here specifically to study cheese[2]. BK assumes cross-relaxation between protein and water and a power-law spectral density due to the protein fractal dynamics[3]. The model was fitted to the NMRD profiles through a three-stage hybrid strategy addressing the practical non-identifiability of the parameters: a coarse grid search, a zoom refinement, and a final simultaneous weighted, regularized nonlinear least-squares fit. Physically motivated bounds and frequency-dependent weighting of the more informative mid- and low-frequency points improved robustness and stability.

The proposed fitting strategy provides a robust framework for extracting physically meaningful MD parameters from FFC-NMRD profiles of a hydrated protein.

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Improving NMR Cryoporometry with Octamethylcyclotetrasiloxane

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NMR cryoporometry is a powerful technique for the structural charazterization of multi-scale nanoporous materials, which relies on the pore-size-dependent shift of the solid-liquid phase transition in confinement[1]. Extending this technique to materials with larger pore sizes would significantly broaden its applicability. However, this requires probe liquids with suitable thermodynamic properties and an accurate interpretation of cryoporometry data that accounts for the influence of pore-network topology and relaxation effects on phase transitions.

In this work, we study octamethylcyclotetrasiloxane (OMCTS), a probe liquid which is of particular interest for probing larger pore materials[2], but its thermodynamic parameters reported in literature exhibit significant differences. Exploiting recent advances in the description of solid–liquid equilibria in confined systems, we develop and apply two independent approaches for determining the thermodynamic parameters of OMCTS. The first approach combines measurements of water and OMCTS in a European reference Controlled Porous Glass material. The second approach relies on OMCTS measurements performed in highly ordered nanoporous alumina membranes with two distinct pore sizes. The two methods yield highly consistent results and the proposed framework establishes a basis for advanced NMR cryoporometry that can be readily extended to other probe liquids, enabling accurate characterization of a broad range of porous materials.

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Kinetic study of rehydration of C-S-H dehydrated by means of water mobility and change in the microporos

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Hydrated cement compounds can be recycled through thermal treatment. There are important gaps in the understanding of the dehydration and rehydration behavior of hydrated Portland cement, which can be addressed by studying the fundamental behavior of the constituent cement phases. Since calcium silicate hydrates (C–S–H) are the phases present in the largest volume (~50–60% of the hydrated products), studying this phase is crucial to understanding and predicting the behavior of recycled cements. The aim of this study was to verify whether it is possible to dehydrate and rehydrate synthetic calcium silicate hydrates (pure phases, obtained by mechanochemical synthesis with Ca/Si molar ratios 0.83, investigating whether the structures of these C–S–H phases remain stable throughout dehydration–rehydration cycle (dehydration at 400 °C for 2 h and rehydration in ultrapure water). The results obtained by the different experimental techniques used (XRD, ATR FT-IR, thermogravimetry) showed that it is possible to dehydrate and rehydrate C–S–H phases produced. Kinetic studies showed that the rehydration phenomenon takes place through direct reformation of the dehydrated C-S-H structure itself, and FT-IR tests evidenced that when rehydrated the C-S-H layers expand as water is imbibed. ^{1}H-NMR shows an instantaneous redistribution of water from coarser pores back into the finer C-S-H spaces to equilibrate internal surface energy gradients because the water controls multiple chemical and mechanical properties of C-S-H.

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Magnetic Resonance Pore Imaging using Simple Echo Pulse Sequences

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Pulsed Gradient Spin Echo methods, as introduced first by Stejskal and Tanner [1], have constantly evolved over time, becoming more versatile and sophisticated. Examples include structural investigations in porous materials, soft matter research, and biomedical applications. More recently, Diffusive Pore Imaging [2], also known as Magnetic Resonance Pore Imaging (MRPI) [3], uses extended gradients to accumulate the phase of the NMR signal as an average over a long diffusion path, thus tracing out pore structures. Achieving the long-time limit for these extended gradients is crucial; otherwise artefacts such as blurring may occur.

Practical implementations of MRPI are challenging because the magnetisation needs to be maintained in the transverse plane for extended periods of time. This is particularly relevant for samples that induce internal gradients due to their heterogeneous internal pore structure. This has previously been mitigated using MRPI pulse sequences similar to CPMG. While this preserves magnetisation, it also introduces complex coherence pathways and requires frequent and rapid gradient switching. Other approaches have used conventional spin-echo sequences, owing to favourable sample structure and alignment in the B0 magnetic field.

Here, we report the use of conventional spin-echo sequences applied to diffusion in glass capillaries with diameters of 20 µm. Even at echo times on the order of seconds, we observed decent signal-to-noise ratios. Depending on the specific properties of the sample being examined, this experimental simplification could expand the applicability of sequences that rely on long diffusion times to media containing closed pores.

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Monitoring Water Populations During White Cement Hydration Using NMR Relaxometry and Dipolar NMR

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Water in cementitious materials plays a fundamental role in the hydration process, the evolution of the microstructure, and the resulting mechanical and transport properties. In particular, water associated with the so-called gel pores, consisting of nanometer-sized spaces between calcium silicate hydrate (C-S-H) nanoparticles, as well as water confined within the interlayer spaces of C-S-H, is severely confined and exhibits molecular dynamics that differ markedly from those of bulk water [1].

Nuclear Magnetic Resonance (NMR) relaxometry is widely employed to investigate the different water populations present in cementitious materials [1,2]. However, the severe restriction of molecular motion experienced by highly confined water makes dipolar NMR techniques particularly well suited to probing these populations. In this context, the present work is motivated by the possibility of combining conventional relaxometry with dipolar NMR methods [3] to simultaneously monitor water populations spanning a broad range of molecular mobilities and degrees of confinement during cement hydration. The experiments are performed on white cement, which serves as a model system because of its low concentration of paramagnetic impurities.

Direct excitation and Magic Sandwich Echo (MSE) experiments [3] are employed to identify and quantify ^{1}H populations associated with strongly confined, low-mobility water species. In parallel, conventional T_1 and T_2 relaxometry is used to monitor the evolution of the more mobile water populations [1,2]. The combination of these complementary approaches enables the simultaneous monitoring of structural water, interlayer water, gel water, and bulk (capillary) water throughout cement hydration, allowing the identification of distinct hydration stages, including the initial and final setting times, as well as the onset of the hardening process.

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NMR and High-Resolution imaging on the MOGNO Beamline for dynamic system analysis on Porous Media

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Time-Domain Nuclear Magnetic Resonance (TD-NMR) stands out for being a non-invasive technique, that allows the measurement of information regarding the molecular dynamics of fluids. In porous media, this technique enables the study of morphological and physicochemical properties of materials, and it is widely applied across scientific and industrial sectors, with current emphasis on CO_2 geological storage [1]. MOGNO is a micro and nano X-ray imaging beamline dedicated to time-resolved experiments (4D tomography) through in-situ experiments, where a material can be observed under specific conditions [2]. Integrating TD-NMR and X-ray imaging is a perfect combination for studies of porous media, mainly under dynamic conditions [3]. It is in this context that the LEAR group at the University of São Paulo, in partnership with the Brazilian Center for Research in Energy and Materials (CNPEM), is developing an TD-NMR system to be installed at MOGNO for simultaneous acquisitions of high-resolution images and NMR data. Data from both techniques will be crucial for understanding the material's evolution and will also complement computational data processing models. Areas involving processes like saturation, imbibition, and flow, including CO_2 capture and storage, soil, cement, and aquifers, can be explored. In addition to areas involving chemical reactions such as porous media acidification. This work will present some aspects of the project that are under development and previously obtained results that will be explored in the future with the combination of both techniques.

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Open-Access Web Application for Inverse Laplace Transform Processing of Time Domain NMR Signals

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Recent advances in compact and low-field time-domain nuclear magnetic resonance (TD-NMR) instruments have considerably expanded their application in food, agricultural, environmental, and materials research. In parallel, the Inverse Laplace Transform (ILT) has become one of the main approaches for extracting relaxation time distributions from TD-NMR signals, providing valuable information about molecular mobility and material structure. However, ILT analysis is still commonly limited to proprietary software or requires specialized knowledge in numerical methods, restricting its widespread adoption by non-specialist users. In this work, we present NMR-ILT, an open-access Web platform for performing ILT analysis of TD-NMR relaxation data through an intuitive and user-friendly interface. The implemented algorithm is based on non-negative least squares (NNLS) combined with Tikhonov regularization and singular value decomposition (SVD), providing robust inversion of ill-posed problems. The platform supports the most widely used TD-NMR pulse sequences, including Carr–Purcell–Meiboom–Gill (CPMG), Inversion Recovery (IR), and Saturation Recovery (SR), and is compatible with data acquired from instruments manufactured by different vendors. The performance of the WebApp was evaluated using simulated datasets and representative experimental signals from food and agricultural materials. The obtained relaxation time distributions showed excellent agreement with those generated by established ILT software while providing a freely accessible, browser-based environment that requires no software installation. By making advanced TD-NMR signal processing openly available, the proposed platform has the potential to facilitate research, teaching, and the dissemination of relaxometry methods across a broad scientific community.

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Quantifying Inter-pore Exchange in Complex Porous Media: A T_2-Filtered NMR Study from Reservoir Rocks to Bioactive Glasses

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Multi-compartment systems are ubiquitous in natural and engineered porous materials, where fluids or ions are distributed among environments with distinct physical, chemical, and geometrical properties. In complex media, ranging from sedimentary rocks with liquid inclusions (e.g., carbonate reservoirs) to mesoporous bioactive glasses, this heterogeneity gives rise to multiple compartments and fluid–surface interactions, which are reflected in broad Nuclear Magnetic Resonance (NMR) relaxation time distributions. However NMR relaxometry does not, by itself, reveal whether these compartments are dynamically connected. In this work, the T_2-filtered T_2-T_2 relaxation exchange method (T_2F-T_2-T_2RE) [1,2] is employed to investigate and quantify the migration dynamics (exchange) of fluid molecules between distinct T_2 environments. This protocol uses a fixed transverse relaxation filter to suppress fast-relaxing components, allowing for a time-efficient tracking of how magnetization is recovered through exchange as a function of storage time. The results demonstrate that T_2F-T_2-T_2RE is able to identify and quantify the exchange rates among pore families, providing a low-field NMR protocol for testing the connectivity of the pore network. In sedimentary rocks, the extracted exchange rates were correlated with macroscopic transport properties, specifically permeability, proving the method's predictive potential. This approach shows significant potential for the characterization of mesoporous bioactive glasses, [3] where understanding the exchange between intra-particle mesopores and the surrounding medium is key to optimizing ion release and drug delivery kinetics. This work highlights the technique's versatility across physics, geosciences, and the frontiers of materials science.

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Study of Local Environments in Crystalline and Glassy Framework Materials by Solid-State NMR

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High-resolution magic-angle spinning (MAS) NMR has become a key technique for investigating porous framework materials, providing atomic-scale information on local structure that complements diffraction by remaining sensitive to short-range order even in highly disordered systems [1]. This capability is particularly important for metal–organic frameworks (MOFs), where amorphization and compositional modifications often preserve local chemical connectivity while disrupting long-range crystallinity.

This contribution presents recent advances in the application of multinuclear MAS NMR to elucidate local structure in crystalline and glassy MOFs. By combining information from spin-1/2 and quadrupolar nuclei, solid-state NMR probes metal coordination, linker environments, chemical connectivity, and structural disorder. In mixed-linker cadmium imidazolate frameworks, ^{1}H, ^{13}C, ^{15}N, and ^{113}Cd NMR demonstrate that vitrification preserves the primary Cd-N coordination network despite the development of local geometric disorder. Complementary ^{113}Cd{^{1}H} REDOR and variable-temperature NMR experiments further distinguish distortions in coordination geometry from changes in chemical connectivity and reveal dynamic processes across the glass transition.

The versatility of this approach is further demonstrated in mixed-metal Zn/Ga ZIF materials. Multinuclear MAS NMR reveals the coexistence of two structural domains after vitrification: a Zn-rich glassy phase and residual Ga-rich crystalline environments. These results show that the local structure and phase evolution can be controlled through metal composition, providing a chemical route to MOF glass-ceramics.

Together, these examples highlight the unique capability of high-resolution MAS NMR to characterize local structure, structural heterogeneity, and glass formation in porous framework materials, providing insights that are inaccessible by diffraction alone.

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Understanding the role of cellulose ether in water retention and hydration process of cementitious tile adhesive using NMR analysis

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Cement-based materials, including Cementitious Tile Adhesive (CTA), are widely utilized for their exceptional binding properties. While the fundamental mechanisms governing their performance are not yet fully understood, workability is known to be primarily controlled by two competing processes: hydration and water evaporation. [1] Studies have demonstrated that cellulose ethers can modulate these processes by reducing evaporation rates and modifying hydration kinetics. [2,3]

This study evaluates the effects of different cellulose ethers and chemical accelerators on two industrial-grade CTA formulations (AC-I and AC-III, respectively, according to ABNT NBR 14081), provided by Saint-Gobain Research Brazil. In the first group (AC-I), hydroxypropyl methylcellulose (HPMC) and hydroxyethyl methylcellulose (HEMC) were tested at concentrations of 0.1, 0.2, and 0.7 wt%. In the second group (AC-III), two types of accelerators were assessed. Water dynamics in the hydration process were monitored using low-field NMR relaxometry (T2 measurements) and one-dimensional MRI (1D MRI).

For AC-I, 1D MRI revealed that increasing cellulose ether creates a drying layer, which is suggested to form an evaporation-reducing barrier. ^{1}H relaxation measurements showed no significant difference between 0.1% and 0.2% concentrations, indicating that evaporation effects in the experimental setup were insufficient to differentiate cellulose retention at low concentrations, although the samples with 0.7% concentration showed a strong chemical reaction retardation and water retention.

In the case of AC-III, ^{1}H 1D-MRI revealed a pronounced difference in the effect of the accelerator during the initial hours of sample curing, enabling the observation of a faster hydration kinetics. ^{1}H relaxation measurements also showed great potential to differentiate the chemical additive effects in hydration kinetics.

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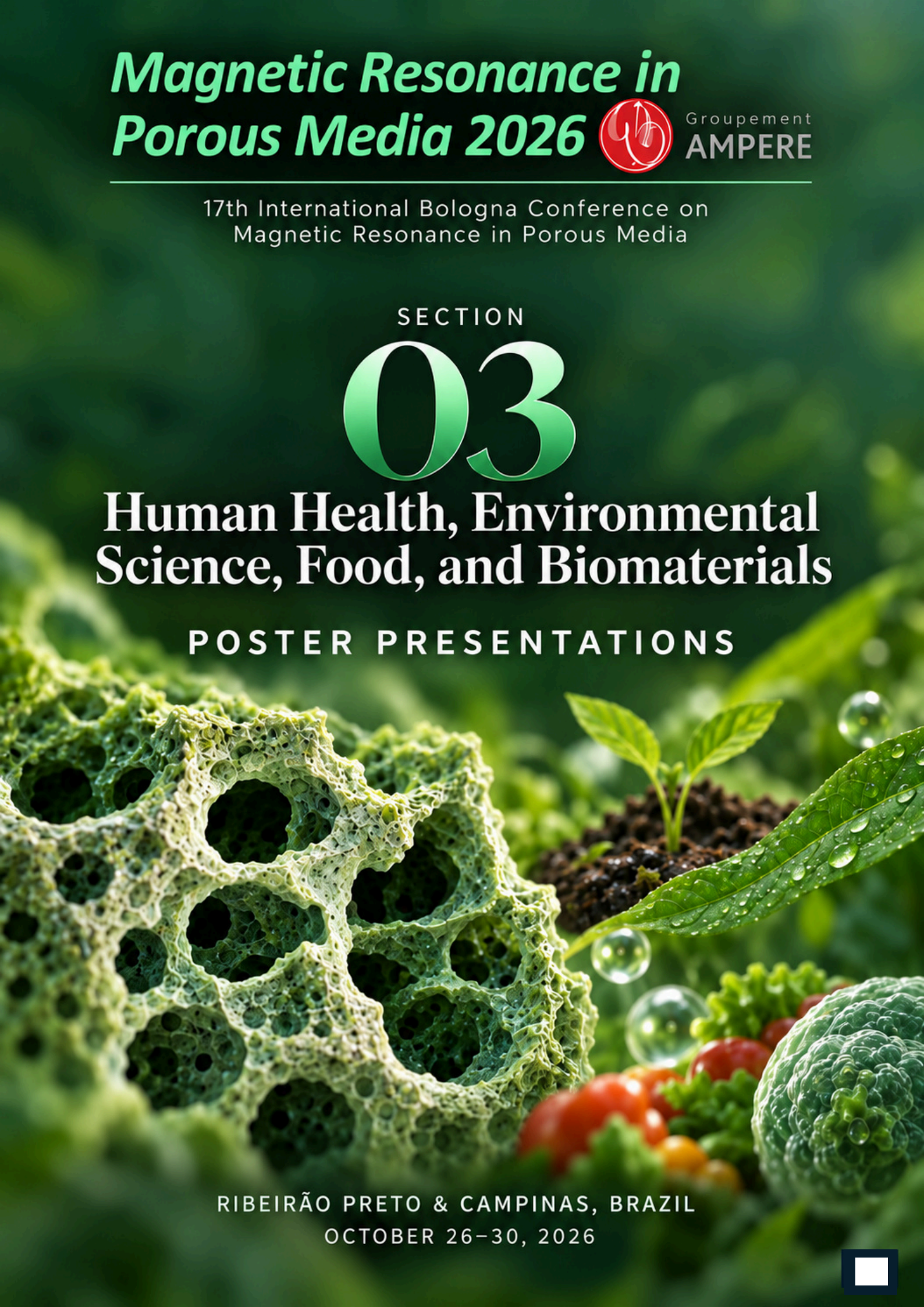
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SECTION

03

Human Health, Environmental Science, Food, and Biomaterials

POSTER PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

OCTOBER 26–30, 2026

Solid-state NMR study of species confined into the nanopores of porous carbon materials

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Porous carbons are widely employed in a broad range of applications, including pollutant removal from aqueous and gaseous media, energy storage devices, heterogeneous catalysis, and CO_2 capture by physical adsorption. Solid-state nuclear magnetic resonance (NMR) spectroscopy is a promising technique for studying molecules and ions confined within the porous network of carbon materials. The main phenomenon observed in the NMR spectrum of a porous material impregnated with a solution is the nucleus-independent chemical shift (NICS). The magnitude of the NICS measured in an NMR spectrum can provide structural information about the porous material under investigation, such as pore size, specific surface area (SSA) and pore volume, among others [1,2]. However, the observation of NICS in an NMR spectrum and its interpretation may be affected by different structural and chemical factors specific to each material studied. Activated carbons (ACs) are porous carbon materials with high SSA and that can be obtained from the pyrolysis and activation of a wide variety of precursors [3]. In this work, ACs produced from the babassu coconut endocarp were impregnated with distilled water and aqueous solutions of NaF, NaBF4, and LiCl for solid-state NMR experiments with magic angle spinning (MAS). The objective was to record 1H, 7Li and 19F NMR spectra and assess the NICS magnitude for the different probe nuclei confined within the porous network. This work seeks to obtain relevant information for understanding the chemical and dynamic aspects of confined species in porous media. The results show that ions of different types exhibit distinct accessibility to the AC porous network, mostly depending on the porosity of the carbon matrix and the ion sizes. In contrast, water molecules readily penetrate the pores of all studied ACs, giving rise to NICS values primarily affected by the pore sizes.

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Study on Human Bone Samples Using Acoustography

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The development of non-destructive methods for bone characterization has become increasingly important for the diagnosis and monitoring of skeletal diseases. Acoustography, based on the detection of vibroacoustic signals generated by ultrasound radiation, has emerged as a promising technique for assessing the mechanical properties of biological tissues. This study aimed to evaluate the feasibility of Pulse Emission Acoustography (APE) for the characterization of human trabecular bone samples and to investigate its correlation with structural parameters previously obtained by micro-computed tomography (micro-CT). Human trabecular bone specimens previously classified as control, osteopenic, and osteoporotic were analyzed using a dedicated acoustography system. A focused 3-MHz confocal ultrasound transducer generated acoustic radiation force, while the resulting vibroacoustic response was detected using a broadband hydrophone. The specimens were scanned using a high-precision three-dimensional positioning system, and the acquired signals were processed to generate acoustographic images. Signal-to-noise ratio (SNR) measurements were obtained from selected regions of interest and compared with previously measured Bone Quality Index (BQI) and structural parameters. Acoustographic imaging successfully differentiated bone specimens presenting distinct structural characteristics. Samples with higher trabecular degradation exhibited lower vibroacoustic signal intensity, indicating reduced mechanical response to the applied radiation force. Quantitative analysis demonstrated a correlation between the acoustographic signal and bone quality parameters obtained by micro-CT. The results indicate that vibroacoustic signal intensity reflects changes in bone microarchitecture and mechanical properties, supporting the potential application of acoustography as a complementary tool for bone quality assessment and osteoporosis research.

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Magnetic Resonance in Porous Media

SECTION

04

Natural and Artificial Porous Media & Cultural Heritage

POSTER PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

OCTOBER 26–30, 2026

Fabrication of Artificial Carbonate Porous Media: A Comparison between Powder Compaction and Additive Manufacturing

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Petroleum engineering utilizes natural rock samples (core plugs) to calibrate characterization tools, such as Nuclear Magnetic Resonance (NMR), and to validate numerical models. However, natural carbonate core plugs are extremely heterogeneous, expensive, and often subject to legal restrictions on their use. There is a significant gap in the production of artificial porous media composed solely of calcium carbonate, as most current replicas rely on polymeric binders or cements that alter the wettability and chemical reactivity of the matrix. This study presents two strategies to obtain pure calcite artificial porous media. The first strategy is isostatic powder compaction using pore-forming agents. This method produces samples with high relative density (up to 93%) and high mechanical strength (up to 110 MPa in compression), which is comparable to natural rocks and sufficient for petrophysical tests under high pressures. Its main disadvantage is geometric limitation to simpler shapes and low permeability (0.05-0.06 mD) due to small, poorly connected pore throats. The second strategy is additive manufacturing (vat-photopolymerization) of calcite with pore formers. The advantage lies in its exceptional geometric freedom, allowing the creation of macroscopic channels and complex structures with fully connected porosity and permeability (30-50 mD). However, the method yields significantly lower mechanical strength and imposes wall-thickness limitations due to the manufacturing process involved. Both methods provide controlled, reproducible porous media for advanced NMR studies. The presentation will compare the two methods, identify which applications are better suited to each, and outline the challenges and opportunities for improvement.

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rocks with multiscale porosity sintered in a CO2 atmosphere. Geoenergy Science and Engineering. 2023;229:212096. https://doi.org/10.1016/j.geoen.2023.212096 .

Factors Influencing Pore Structure Changes in Purple-clay (Zisha) Ceramics: A Comparative Study Using 1H NMR Relaxometry and Mercury Intrusion Porosimetry

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Single-sided nuclear magnetic resonance (NMR) offers a non-destructive approach for characterizing the pore size distribution in porous ceramic materials[1]. In this study, we applied single-sided NMR to investigate the pore structure of Purple-clay (Zisha), a mineral-based ceramic clay traditionally used for the production of teapots and provide relatively sweeter tea soup[2]. This special effect is thought to be possibly related to the pore structure inside Purple-clay[3], but so far it has not been fully investigated. We studied Huanglongshan-Dicaoqing Purple-clay from Dingshu Town, Jiangsu Province, and compared it with a commonly used soil-based clay from Meishan Town, Zhejiang Province. We also evaluated the influence of traditional clay preparation versus modern machinery-based preparation.

The pore size distribution was investigated using 1D and 2D NMR time-domain measurements performed with a MOUSE PM10 device (Magritek, New Zealand; B_0 = 0.327 T). Complementary mercury intrusion porosimetry measurements were performed using ThermoQuest instruments from the PASCAL 140 and 240 series to support the interpretation of the porous structure derived from NMR. The results show that Purple-clay materials have a higher percentage of pores in the 20–150 nm range compared to normal soil-based clay, providing quantitative evidence of their different porous architecture. Traditional clay preparation further increased the proportion of larger pores and produced a continuous pore size distribution. These results demonstrate that single-sided NMR can serve as an effective quantitative tool for evaluating the porous structures of Purple-clay and for distinguishing the material’s provenance and preparation method.

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Oleogel assembly and application: from a porous-media characterization to a biofertilizer technology

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An oleogel is, by definition, a 3D structure created by incorporating a structuring agent, known as a gelator, which forms self-assembled structures via physical bonds, encapsulating a hydrophobic liquid. This enables the formation of a porous media containing micelle-like structures in its makeup, physically enclosing the oil within the structure. Time Domain Nuclear Magnetic Resonance is a versatile technique for material characterization, providing insights on its properties and structure. Although sequences of transversal relaxation measurements, such as CPMG, are commonly employed for this purpose in oleogel samples, longitudinal relaxation and Magic Sandwich Echo (MSE) techniques remains unexplored. These are valuable methods due to their ability to quali- and quantitatively access interactions, viscosity, and material structure. The present study ensabled an oleogel structure and explored such sequences to characterize it. In addition, it tests an application of the final material as a biofertilizer for a bacterial biopesticide.
Using Ethylcellulose as structuring agent, it was possible to obtain a physical entanglement with the Soybean oil (SO) through hydrogen bonds. This enabled the organization of a gel-like porous material. It was oberserved a relationship between concentration increase and a progressive self-organized structure, with more brittle forms at even higher concentrations. The T1 and T2 sequences revealed a limitation in molecular mobility as the concentration increased, leading to the development of micelle-like structures. Conversely, the MSE successfully quantified the Rigid fraction (Rif) and detected an excess in the Rf, implying the immobilization of the SO. Meanwhile, when evaluating the feasibility of such material as an encapsulating agent for controlled release of Bacillus thuringiensis as biopesticide, it was possible to demonstrated its ability to extends cellular viability during both storage and field-application conditions.

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Water Absorption and Dynamics in 11th Century Wall Paintings: Assessing Surface Treatments via NMR Profiling

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In-situ NMR depth profiling for cultural heritage purposes is an expanding field[1] due to its advantages over most other techniques which are limited to surface analysis. Specifically, when investigating the water absorption properties of surfaces, NMR can directly characterize both water content and its kinetics[2,3] using portable and low-cost equipment.

This study investigated 11th century wall paintings in the Collegiate Church of St. Pietro and Orso in Aosta via single-sided NMR depth profiling, using an NMR-MOUSE PM10 (B_0 = 0.327 T) mounted on a micrometric precision lift. This work aimed to evaluate and compare the removal of hydrophobic coatings using methyl ethyl ketone (MEK) applied via two innovative electrospun tissues. Eight measurement spots were selected to account for potential variations in the cleaning process caused by pigment composition and uneven coating distribution.

Before and after treatment, each spot was profiled three times using CPMG sequences after moistening with a spray dispenser. The first profile, acquired immediately after spraying, was used to set the depth range for the subsequent profiles, which were acquired after 20 and 40 minutes. Noise profiles were collected to filter the signal, along with a weighted moving average between subsequent profile points. The analysis focused on the cumulative profiles and their slopes, which respectively represent the total water content and its spatial distribution.

Both cleaning methods were confirmed to remove the hydrophobic coating, given that faster water transport was observed. The analysis also showed one carrier tissue predominantly increasing the total volume of water penetrating the wall surface, whereas the other promoted a more homogeneous spatial distribution. These results confirm single-sided NMR as a powerful tool to investigate the structure of porous media of interest to cultural heritage whose standardization would lead to procedures accessible to non-NMR experts.

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Water dynamics and structural evolution in silicate-based porous media: from solutions to colloidal gels probed by dynamic NMR relaxometry

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Understanding water dynamics in porous media, from reactive solutions to consolidated gels, is essential for predicting transport, aging, and stability in natural and engineered materials. However, capturing these processes under non-equilibrium conditions across relevant time and length scales remains challenging.

In this work, we develop and apply a dynamic low-field NMR relaxometry framework to investigate water dynamics and structural evolution in silicate-based systems, spanning from alkaline solutions to deformable colloidal gels.

We first investigate aqueous alkali silicate solutions to quantify changes in water mobility and interfacial interactions as a function of hydroxide concentration and alkali nature. Transverse relaxation measurements show that NMR relaxometry provides a sensitive probe of solution speciation and early-stage mesoscale organization, even prior to gel formation.

We then extend this approach to drying colloidal and aluminosilicate gels, where water transport is coupled to deformation, gradient formation, and network reconfiguration. By tracking transverse relaxation times (T_2) as a function of saturation, and combining bulk measurements with one-dimensional spatial water profiles, we identify power-law relationships linking relaxation efficiency and desaturation. These relationships reveal distinct drying regimes and enable discrimination between homogeneous and instability-driven drying.

A minimal numerical framework is introduced to separate the contributions of gradient development, macroscopic contraction, and particle network reconfiguration. Overall, this work establishes NMR relaxometry as a unified, non-destructive tool to probe water dynamics in evolving porous media.

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SECTION

05

Mobile NMR

POSTER PRESENTATION



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

OCTOBER 26–30, 2026

Designing and Shimming Halbach Array Magnets: A Historical Perspective with Modern Implications

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Most magnetic resonance practitioners developing or using array (or ring) magnets refer to them as “Halbachs” and almost always reference Klaus Halbach’s 1980 paper. However, evidence suggests that modern workers rely heavily on magnetic field simulation software and are largely unaware of most of the theoretical results in the paper. This may be due to the terse presentation of the unfamiliar complex-valued techniques used by Halbach.

Even more under-utilized is the work of Bob Gluckstern from the mid-1980s. He developed methods for calculating and mitigating the effects of finite length in these magnets. Unfortunately, his results are publicly available only in abbreviated and cryptic form in a patent. The details of Gluckstern’s work are known only to those who worked directly with him.

The early work of Halbach and Gluckstern was done mostly with pencil and paper. It is rich with insights that may be obscured by computer simulations and calculations. We continue to use the techniques to design and build magnets, and it strikes us that familiarity with these 40-year-old results would be beneficial to modern magnet designers, especially those seeking higher homogeneity.

To that end, we present the nearly lost theory in some detail. We work a number of practical examples and discuss implications for magnet design projects. We hope that even those who are not currently designing magnets will recognize the importance and value of acknowledging the giants of our field.

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Revisiting Shim-a-Ring Magnets for Improved *B* Homogeneity

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Halbach magnet assemblies are widely used in NMR to generate strong static magnetic fields with good field homogeneity within the sample region while minimizing external stray fields [1]. In practice, these assemblies are realized using multiple discrete magnet segments with prescribed orientations [2], leading to significant fabrication complexity, sensitivity to tolerances, and bulky structures.

The “shim-a-ring” magnet [3] provides a simpler alternative based on a single diametrically magnetized ring and a concentric ferromagnetic shim. The induced magnetization of the shim follows the spatial field distribution of the ring, resulting in an effective continuous angular variation analogous to an ideal Halbach configuration. This architecture supports straightforward, self-aligned assembly without the need for precision placement of multiple magnets. Despite these advantages, the shim-a-ring approach is constrained by limited degrees of freedom for shaping the magnetic field, which can restrict achievable field homogeneity compared to discretized assemblies.

In this study, we extend the shim-a-ring concept by introducing refined configuration strategies that improve control of the magnetic field distribution while preserving simplicity and compactness. Representative analyses demonstrate that enhanced ring-based designs can achieve improved field homogeneity without the complexity of multi-element magnet assemblies, supporting the development of practical permanent magnet solutions for compact NMR systems.

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TD-NMR in Semicrystalline Polymers: Morphology and Dynamics

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Time-Domain NMR (TD-NMR) is particularly well suited for probing phase composition, molecular mobility, and nanoscale morphology in semicrystalline solids due to the dominance of the dipole-dipole interactions. TD-NMR is especially valuable for investigation of structurally complex systems, composed of phases with distinct molecular mobility. In this work, commodity polymers (polyethylene and polypropylene) with various crystallinities are investigated using several TD-NMR experiments over a wide range of temperatures. The analysis of the FID and related sequences based on the second-moment approximation allowed identification of thermal regions with uniform relaxation behavior. The temperature dependence of the spin-lattice relaxation revealed characteristic extrema associated with different motional regimes, from localized side-group reorientations to cooperative segmental chain dynamics.
Additionally, the double-quantum and multiple-quantum NMR experiments were used to gain information about the structural heterogeneity obtained from distributions of residual dipolar couplings, which reflect local motional restrictions of crystalline and amorphous phases.
Finally, the nanoscale morphology was characterized by spin diffusion experiments, which probe magnetization transfer between domains of different mobility. Using data from DQ experiments, we demonstrated the possibility to estimate domain sizes while avoiding spectral deconvolution.
Overall, the utilization and analysis of variety of available TD-NMR techniques provide a unified, model-free framework for describing crystallinity, molecular mobility, and phase morphology in semicrystalline polymers. TD-NMR thus delivers comprehensive structural and dynamic information across multiple time and length scales in complex polymer systems.

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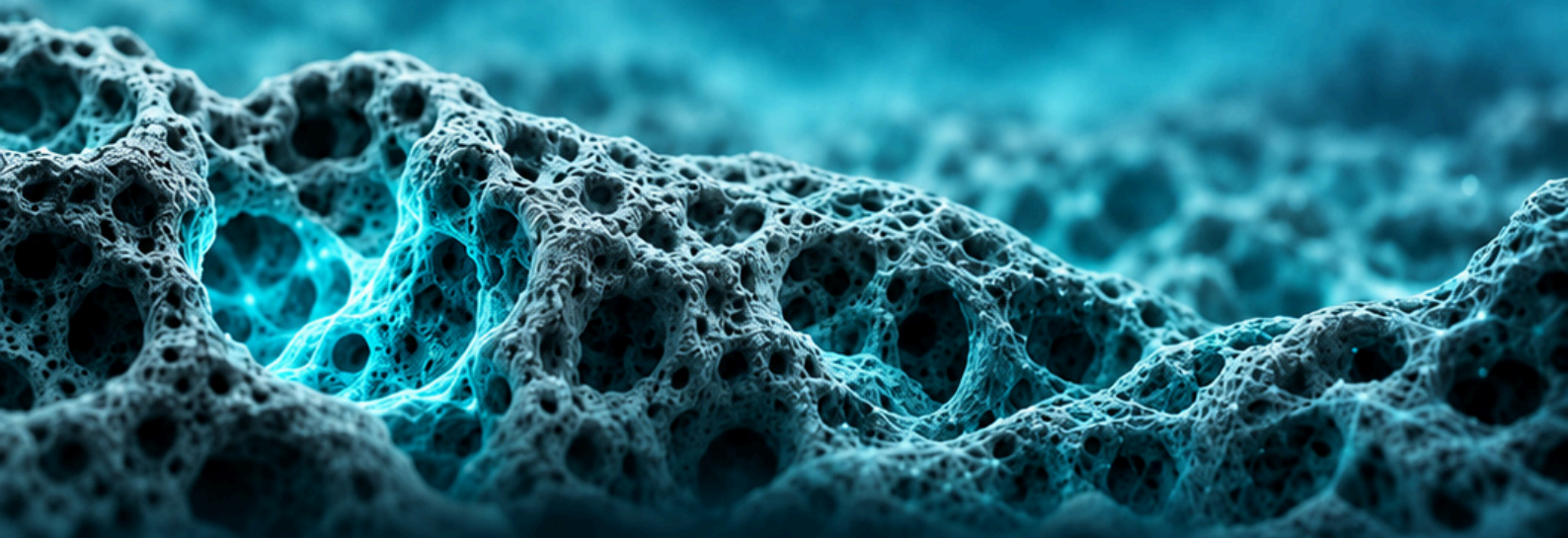
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SECTION

06

Advances in Mathematics, Engineering, AI, and Quantum Computing

POSTER PRESENTATIONS



RIBEIRÃO PRETO & CAMPINAS, BRAZIL

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Acoustic Techniques for Porosity Analysis in Petroleum Reservoir Sandstones

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The characterization of oil reservoir rocks is critical for the petroleum industry, as porosity, permeability, and mineral composition directly determine fluid storage and flow. Conventional methods like scanning electron microscopy, X-ray diffraction, X-ray microtomography, and nuclear magnetic resonance are accurate but costly, slow, and complex. To address this, the research investigated photoacoustic microscopy (PAM) and vibroacoustography (VA) for sandstone rocks. PAM uses pulsed laser absorption to generate acoustic waves encoding optical and mechanical properties. Using a 532 nm laser, PAM images of 11 sandstones were acquired, with porosity from 18.8 to 32.8% and pore radii from 6 to 60 µm. Signal intensity was compared with photographs to identify mineral regions. Brighter PAM regions corresponded to higher absorption, and k-means clustering achieved Lin's concordance of 0.972. Frequency analysis showed mean frequency correlated with pore radius (Spearman -0.81, R^2 0.80), while porosity correlation was weaker (-0.41, R^2 0.26), indicating pore dimensions dominate acoustic response. VA is based on nonlinear interaction of two confocal ultrasound beams at different frequencies, generating lowfrequency signals sensitive to stiffness and porosity. Experiments on alumina ceramics (5–30% porosity) showed linear VA amplitude increase in the 82–85 kHz band. For sandstones, VA followed this trend, except Berea and Boise due to mineralogical differences, revealing sensitivity to heterogeneity. VA images also showed hot spots in porous samples, suggesting mechanical variations. Both techniques are non-contact, lowcost, and operate in reflection mode, suitable for field use. However, reservoir heterogeneities over centimeters to meters scales mean small plugs may not represent bulk formations without upscaling. The findings demonstrate that PAM and VA are promising complementary tools for porosity estimation and morphological analysis of reservoir rocks.

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An NMR Platform for Quantum Computing

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NMR remains one of the most versatile techniques for demonstrations of quantum computing. In this work, we present Ugly-Cat, an experimental-computational platform utilizing the quadrupolar coupling of ^{23}Na nuclei in a liquid crystal sample placed in a 9.4T magnet. (1,2) The four energy levels of this quadrupolar nucleus directly form a 2-qubit Hilbert space, without requiring multiple coupled spins. Starting from thermal equilibrium, the computational basis states are prepared using strongly modulated rf pulses (3). These pulses are numerically optimized by varying the amplitude and phase while incorporating the quadrupolar Hamiltonian into the optimization to achieve high-fidelity state preparation. Similarly, the components of the universal set of quantum gates, such as Hadamard gates, are prepared using the same rf pulse optimization approach to generate, for example, the entangled states required for the implementation of basic quantum algorithms. The platform also simulates the time evolution of the quantum system, enabling prediction of the quantum states produced by any pulse sequence. These states can be experimentally reconstructed using quantum state tomography (2), which yields the full density matrix and allows the fidelity of the implemented quantum operations to be quantified. The entire pipeline is integrated into a graphical user interface (GUI) where users can draw arbitrary 2-qubit circuits. The system automatically compiles these circuits into rf pulse sequences, executes them on the spectrometer, and displays the experimentally reconstructed state alongside the simulated prediction, making the platform highly accessible to non-NMR experts. The same architecture is being extended to a 3-qubit system using ^{133}Cs nuclei in a liquid crystal sample. As a next step, we aim to advance quantum computing methods for signal processing, targeting future applications in porous media using in-house NMR systems or higher-qubit commercial quantum processors.

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Deep Learning Analysis of T1-Weighted MRI for Characterizing Vertebral Fragility

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Introduction: Bone strength transcends mineral density, depending on trabecular microarchitecture and marrow adipose tissue. While DXA is the standard for osteoporosis diagnosis, its 2D projection often misclassifies fracture risks. MRI offers a non-invasive 3D evaluation of the bone's porous media. We investigate the computational analysis of T1-weighted lumbar spine MRI using Convolutional Neural Networks (CNNs) to identify bone fragility.

Methods: A dataset of 1,773 vertebral body images was extracted from T1-weighted MRIs of 59 females. Patients were stratified by DXA and fracture history: Normal, Osteopenia (with/without fracture), and Osteoporosis (with/without fracture). After applying Contrast Limited Adaptive Histogram Equalization (CLAHE), we evaluated CNN architectures (ResNet50, MobileNetV2, VGG16). VGG16 with partial fine-tuning was selected to extract high-frequency spatial patterns representing trabecular disorganization and fat infiltration.

Results: VGG16 demonstrated superior performance in capturing the textural signature of the porous tissue. In binary classification, it distinguished normal bone integrity from osteoporotic fragility with an AUC of 1.00. Crucially, it revealed a phenotypic convergence: images of osteopenic patients with fragility fractures shared the exact visual and textural patterns of severe osteoporosis. PCA of the latent space confirmed this, polarizing samples into distinct extremes (Integrity vs. Fragility Signatures).

Conclusion: CNN-based MRI texture analysis captures the structural quality of the porous trabecular network, prioritizing biological risk over pure densitometry. VGG16 applied to routine T1-weighted MRIs acts as a sensitive complementary biomarker, offering a pathway for automated opportunistic screening of vertebral fragility.

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Ugly Cat, a computational system for Quantum Information processing based on NMR

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A modular computational platform, denoted Ugly Cat, for operating the NMR-based Quantum Information processing machine developed by LEAR [1], is presented. The integrative core of Ugly Cat platform orchestrates the dynamics of the modules required for operating the Quantum Computer, for producing radiofrequency (rf) pulses necessary for the creation of quantum states, and for feeding the visual interface. A module based on Krotov algorithm for quantum control produces rf pulses of specific intensity, duration, and phase to generate initial states or logic gates in the Quantum Computer.

The Hamiltonian used to define the control consists on coupling the nuclear spin with the external fields through: (i) the Zeeman interaction (dominant term); (ii) the quadrupolar interaction (time-independent perturbation); (iii) the radio-frequency pulses (time-dependent perturbation). The propagator is used to compute spin system time evolution under the aforementioned interactions.

A module for translating rf pulses into commands for an NMR console was developed. A module for visual interface (based on Quirk package [2]) enables drag-and-drop design of quantum circuits along with their respective simulation and experimental evaluation in a NMR-based Quantum Computer.

A module translating the output of the NMR machine into visualizable quantum states was produced.

The modular structure of our platform allows it to be adapted for operation with any NMR spectrometer console, as well as other classes of Quantum Computers, including those based on Nuclear Quadrupolar Resonance (NQR) [3].

As the next step, our research groups will advance quantum computing protocols to improve signal processing, utilizing the two- and three-qubit NMR/NQR systems we have developed.

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