Final report on PD OTKA project 135169

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In the three years of my PD-OTKA project the progress of the experimental work followed the original workplan, and was completed with several new ideas and directions. In the following I sum up the scientific results for carbon-based materials and clay minerals, the methodological achievements and collaborations that were gained during the project. Beside numerous conference presentations, the following six scientific papers were published open-access during the project, being referred later in the report. Further promising results, being before publication, are presented in more details.

1. **Kéri M**.*, B. Nagy, K. László, I. Bányai, Structural Changes in Resorcinol Formaldehyde Aerogel seen by NMR, Microporous and Mesoporous Materials, Vol. 317, 2021, 110988, IF: 5.876, Q1.
2. **Kéri M.***, D. Nyul, K. László, L. Novák, I. Bányai, Interaction of resorcinol-formaldehyde carbon aerogels with water: A comprehensive NMR study, Carbon, Vol. 189, 2022, p. 57-70, IF: 11.307, D1.
3. Nyul, D., Novák, L., **Kéri, M**. and Bányai, I., A Simple Elimination of the Thermal Convection Effect in NMR Diffusiometry Experiments, Molecules 27(19) 2022, IF: 4.927, Q2/Q1.
4. V. Papp, R. Janovics, T. P. Kertész, Z. Nemes, T. Fodor, I. Bányai, **M. Kéri***, State and role of water confined in cement and composites modified with metakaolin and additives, Journal of Molecular Liquids, Vol. 388, 2023, 122716. IF: 6, Q1.
5. L. Wylie, **M. Kéri**, A. Udvardy, O. Hollóczki, and B. Kirchner: On the Rich Chemistry of Pseudo-Protic Ionic Liquid Electrolytes, ChemSusChem, 16 1-14, 2023, IF: 8.4, D1.
6. Váradi B. N. Lihi, S. Bunda, A. Nagy, G. Simon, **M. Kéri**, G. Papp, G. Tircsó, D. Esteban-Gómez, C. Platas-Iglesias, F.K. Kálmán, Physico-Chemical Characterization of a Highly Rigid Gd(III) Complex Formed with a Phenanthroline Derivative Ligand, Inorganic Chemistry, ACS, 61(34) (2022), 13497-13509, IF: 5.436, Q1.

Carbon-based materials:

- Carbon aerogels are prepared from resorcinol formaldehyde organic aerogels, having large specific surface area and micro- and mesoporous structure. Since the applications of carbon aerogels mostly happen in wet form, **NMR cryoporometry was employed to follow the porous behavior of an organic aerogel and its carbon derivative**, as well as the textural changes after the pyrolysis. In the polymer aerogel, saturated with water, by NMR we found spherical mesopores confined by the aerogel beads and wide channels in the macropore size-range separating the aggregated beads. After

carbonization cylindrical pores were observed between the beads and the aggregates got closer to each other. On the other hand, the hydrophobic cyclohexane probed exclusively the macropores, which might be the result of local swelling. The micropore region both in the polymer and the carbonized form was explored only by the low temperature gas adsorption measurements. [1]

- I investigated and compared **the morphology of resorcinol-formaldehyde carbon aerogels synthesized in different ways with a complex use of NMR methods, while their pore structure was stepwise saturated with water**. The wetting properties were studied by vapor adsorption and low-field NMR relaxometry, while the morphology was followed by NMR cryoporometry during the hydration process. At several water saturation levels, the self-diffusion of water was measured. The comprehensive evaluation of the results led to a **detailed description of the wetting process** of these carbon aerogels beyond the pore size distributions. At low hydration level water clusters formed on and around the hydrophilic functional groups of the surface being able to adsorb water, but no continuous water layer developed on the surface. With increasing water content, spherical water drops formed inside the pore system, and vapor phase diffusion was observed in the partially filled pores. Subsequently the interconnected pore structure was saturated. With these results, it was clearly shown that the presence of ionic liquid in the initial solvent mixture increases the surface density of hydrophilic functional groups, reduces the amount of micropores and affect the structure of the resulting carbon aerogels. These results were published in a high-impact scientific journal, which publication won the **Publication of the month (May 2022) prize of the Hungarian Academy of Sciences** as well as the **Publication Award of the Count István Tisza Foundation for the University of Debrecen (2023)**.[2]
- According to NMR cryoporometry the morphology of carbon aerogels in aqueous medium can be tuned by the ionic liquid (IL, 1-ethyl-3-methylimidazolium ethylsulphate, Emim $EtSO_4$) content of the initial mixture during the synthesis. Furthermore, relaxometry data have shown, **that the surface properties of the pores and also the polydispersity are altered by the IL**. To understand this effect and the change of the surface chemistry, high-field NMR experiments were carried out on the monomer/IL/water solutions during the early stages of the aerogel synthesis. Conclusions were drawn on the strength of interaction between resorcinol and the imidazolium ring and aliphatic protons of the ionic liquid. After formaldehyde addition NOESY NMR spectra showed **very strong connection between the formed prepolymer and Emim**, which can contribute to the ability of IL to alter the polymerization process and the accessibility of O-functionalities. This finding was further supported by molecular dynamic calculations of the interaction between the prepolymer and the IL ions by Prof. Oldamur Hollóczki (Dep. of Physical Chemistry, University of Debrecen). The results were presented as a poster in the *CPBCI conference* (2022) as well as in the *Alpine NMR Workshop* (2023) and *CESEP (Carbon in the changing world) Conference* (2023) as oral presentations, and is the topic of a manuscript under preparation **(D. Nyul, I. Bányai, O. Hollóczki,**

K. László, M. Kéri*: Structure-directing effect and surface modifying properties of ionic liquid in the synthesis of RF carbon aerogels, manuscript before submission).

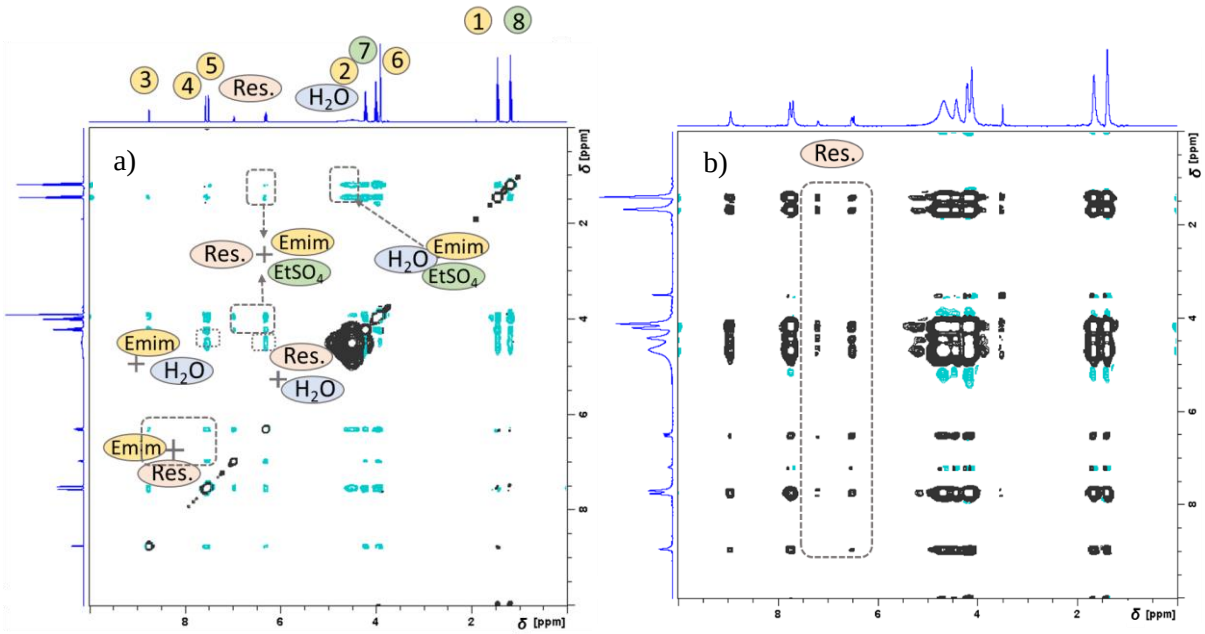

Fig. 1. ^{1}H NOESY NMR spectra of resorcinol dissolved in Emim-$EtSO_4$-water mixture (at highest IL ratio) (a), and the prepolymer after 2 days polymerization reaction with formaldehyde at 80°C (b) (400 MHz, mixing time 800 ms).

– P**olymer and carbon aerogels were synthesized in different ways** and their morphology was described using NMR relaxometry, cryoporosimetry and diffusometry. With these methods we can show how the temperature, the catalyst, the monomer concentration and the composition of the starting solvent mixture affect the structure of the resulting carbon aerogels immersed in liquid. Preparation at lower temperature increases the porosity and hydrophobic feature of the surface. **Cryoporometry and relaxation measurements were carried out in water and cyclohexane, a polar and a non-polar test liquid**. The measurement of the T_2 relaxation time constant of the pore-filling liquid showed the process of filling the pores: water molecules form clusters on the hydrophilic functional groups of the mesopores and fill the pores one after the other, while cyclohexane forms an adsorbed layer on the hydrophobic surface and gradually fills the larger pores. Interestingly, using **cyclohexane improved the resolution of the pore-size distribution compared to water (Fig. 2a-b), while immersion in water revealed pores of the same size with different surface properties**. NMR cryoporometry curves were obtained with a mixture of water and cyclohexane, to parallelly detect the phase transitions and observe the wetting of the porous structure by the two liquids of opposite polarity. This way of studying **competitive adsorption, the spatial distribution of the adsorbates** is obtained beyond the adsorbed amounts. It was clearly observed that the smallest amount of cyclohexane is able to displace water from the mesopores (Fig 2c.).

These results on the spatial distribution of the hydrophilic functional groups and on such behavior of carbon-based adsorbents is going to form a later publication about the manner and extent of removing non-polar environmental pollutants from aqueous medium.

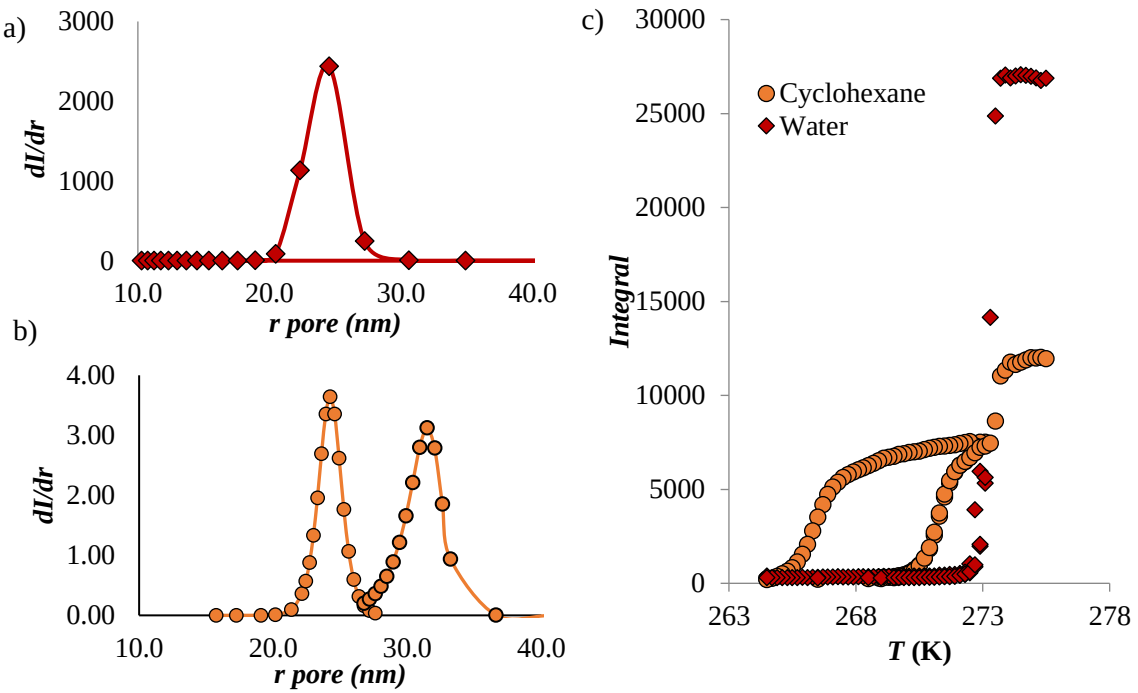

Fig. 2. NMR cryoporometry pore size distributions of a carbon aerogel immersed in water (a) and cyclohexane (b). Freezing and melting curves of cyclohexane and water in a carbon aerogel, showing cyclohexane transition processes in mesopores while water freezing and melting at bulk transition temperature. (c)

- When carbon aerogels are used as adsorbents, an important question is whether **cations bind on the surface of the aerogel**. The T_2 relaxation of the quadrupole sodium nucleus in the pores of the aerogel filled with NaCl solution did not indicate the adsorption of Na-ions.
- I studied **graphene oxide and reduced graphene oxide samples** (synthesized by Prof. Krisztina László, BME) by NMR relaxometry with the aim of revealing the state of adsorbed water on the O-containing functional groups of the surface at several relative humidity values. The results show definite difference between the samples prepared with chemical and thermal reduction in the surface properties, and provide information about the distribution of water between the different functionalities during water vapor adsorption.
- **Graphene-oxide was incorporated into a porous resorcinol formaldehyde polymer aerogel** (see SEM image, in Fig 3, showing the aerogel structure and the graphene oxide sheets). The morphological study of this hybrid aerogel showed micro- and mesopores by nitrogen gas porosimetry, and high mesoporosity with cyclohexane test liquid by NMR cryoporometry (Fig.3). XPS analysis revealed C=O, C-O-C, C-OH functionalities on the surface. The graphene oxide sheets

enlarge the specific surface and enable the connection of functional groups to the structure, while the aerogel skeleton prevents the adhesion of the graphene oxide sheets. The potential application was tested by **Cu(II) ion adsorption** experiments, where the adsorption capacity reached 250 mg/g.

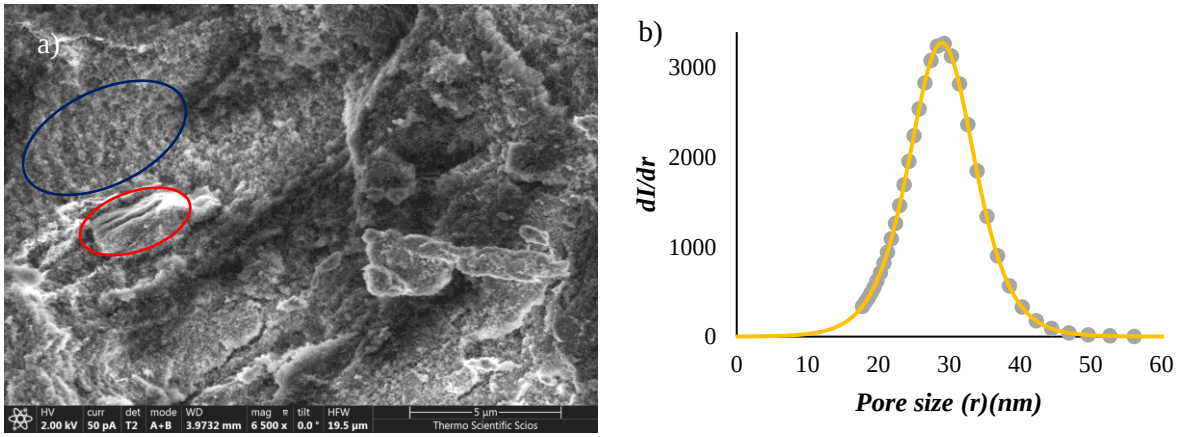

Fig. 3. SEM image (a) and pore size distribution from NMR cryoporometry freezing process assuming cylindrical pore geometry (b) for a graphene-oxide containing carbon aerogel.

Clay minerals:

- Clay minerals, as naturally occurring porous materials, are able to swell in aqueous medium and bind ions in the interlayer space. One of the objectives of the project was to use NMR to investigate the differences in the hydration of montmorillonites containing different counterions. The degree of swelling and the types of water in the structure can be easily monitored with NMR relaxometry. In water-saturated Na-montmorillonite **slit-shaped pores** of approx. 9 nm wall-distance were reproducibly **detected by NMR cryoporometry**. For Ca-montmorillonite 10-12 nm was obtained for the same size. It is not easy to carry out such experiments on the layered structure of clay minerals, as the melting point of the water inside the pore is the same as that of the bulk phase, only freezing point depression occurs, which is difficult to measure due to the supercooling of water in the pore system.
- **Diffusion of water is more restricted in swollen Na-bentonite than in Ca-bentonite**. From the diffusion time dependence of diffusion coefficients, the **mean free path of water molecules** in swollen Na-bentonite is 6-8 µm depending on the water content. According to the literature due to the osmotic swelling of Na-bentonite the diffusion is restricted, resulting in shorter free path. The lack of this type of swelling allows faster diffusion, and longer path (16-26 µm) in Ca-bentonite. Diffusion and pore-size data are before publication along with further diffusion results measured by the NMR MOUSE.
- By T_2 transverse relaxation time constants the **water domains in the layered structure were identified** both for Na- and Ca-bentonites. The change of different water domains was followed

during the saturation and the connectivity between different compartments was characterized in the pore network. I also contributed to the elaboration of a method based on T_2 relaxometry an chemometrics for the determination of the ratio of Na- and Ca-montmorillonites in natural rocks, which is a part of the PhD thesis of Máté Csontos and is before publication.

- **The diffusion time-dependence of diffusion coefficients** gives information about hindered or restricted diffusion and the permeability of the measured system. In some special cases we found increasing diffusion coefficients with diffusion time, which was explained with the **effect of thermal convection** and experimentally confirmed. The extrapolation of diffusion coefficients to zero diffusion time can be a solution for the elimination of this technical problem. [3]
- The original research plan contains the **NMR study of H-bentonite samples** to show the impacts of the acidic treatment on soils. However, studying the pore size by cryoporometry in clay minerals is difficult, while diffusion measurements were neither easy to be carried out because of the fast relaxation of water molecules in the pores. Furthermore, the pore structure of H-montmorillonite seemed to be destroyed from preliminary Cu(II) adsorption measurements. For these reasons the more detailed study of H-montmorillonite was not executed contrary to the original research plan.
- While clay minerals are used as an engineering barrier in the construction of radioactive waste disposals, the waste itself is conditioned in cement containing metakaolin to immobilize radioactive ions during the treatment process. **Metakaolin, a heat-modified alumino-silicate clay mineral**, is applied as an additive to the cement in the conditioning process in the radioactive waste disposal. It improves the physical properties of cement and adsorbs the radioactive ions and basic compounds of the waste. By NMR relaxometry and cryoporometry **the water and pore types were clearly identified in the hydrated pure metakaolin and also in the metakaolin containing cement**. For the accurate determination of the effect of metakaolin on the cement structure, the hydration process of the binders and the hardened structure were characterized. Over the hydration process the **formation of the solid structure is faster in the case of the metakaolin containing cement composite**, due to the precipitation of larger amount of Calcium-Silicate-Hydrate gel. The T_2 transverse relaxation time distribution showed that the **metakaolin is built into the CSH gel structure** of the formed cement stone, and do not alter the nanostructure of the CSH region. However, it significantly decreases the size of the large capillary pores, confirming the expected structural improvement of the binder. The more compact structure **hindered the diffusion of water** within the system, which was inferred from the magnitude change of the determined diffusion coefficients. These results also demonstrate that the applied nuclear magnetic techniques can be effectively applied in the structural analysis of hydrated clay and cement materials as well as in the characterization of water mobility in the solid matrices, thus these methods can contribute to the optimization and development of proper binders for the final disposal of radioactive waste. [4]
- With the use of alumino-silicates, like metakaolin, geopolymers can be synthesized by alkaline dissolution in the presence of extra silica source. **Geopolymers can be novel binders in the**

condition process of radioactive ion-exchange resins. Under my supervision, Vanda Papp PhD student prepared metakaolin-based geopolymer samples and successfully tested its applicability as a binder. The maturation process of the geopolymer was followed by NMR T_2 relaxometry which proved to be a perfect and novel way for the detailed characterization of the process (Fig. 4).

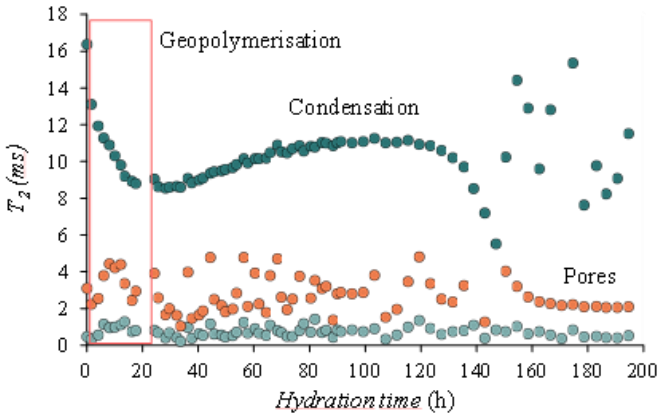

Fig. 4. T_2 relaxation constants as a function of curing time during the binding of a metakaolin-based geopolymer.

– NMR relaxometry is often used in geology to evaluate the **water-retaining capacity of rocks**. The so-called cut-off value serves for the determination of the „free fluid index" and the „bulk volume irreducible", meaning mainly the clay-bound water. These values are essential to estimate the reservoir rocks applicable for the long-term storage of high-level activity nuclear wastes. For potential siltstones our instrument was optimized for such measurements and **the determination of the cut-off value was implemented with a mathematical transformation of the relaxometric data**. It became clear, that for materials where several water types are formed during hydration only the inverse-Laplace transformation of the primary data is worth to be applied. The **surface mapping** of siltstone boreholes was also implemented by the NMR MOUSE.

Methodological and technical achievements:

– **Corroboration and comparison of NMR cryoporometry with the conventional pore size determination methods**: Through the comparative analysis of an RF polymer aerogel and its carbon aerogel derivative, we found similarities and differences, when using the widely applied and well-standardized low temperature nitrogen adsorption method (in vapor phase) and the recently adapted NMR cryoporometry technique (in liquid phase, water and cyclohexane were used as polar and non-polar immersion media). It was confirmed that the two methods provide complementary information about the texture of the investigated porous systems. The microporous region can be explored by N_2 adsorption, in the mesopore size-range both techniques provide similar pore size distribution, while

NMR cryoporometry expands the observation limit toward the macropore region. The combined application of the two methods allows a more detailed structural study of porous materials including the structural changes resulted from the carbonization in the case of carbon aerogels and the occasional change of the morphology caused by the probe liquids.[1]

- **Routine use of cryoporometry for the pore size and shape analysis** of porous materials. **NMR cryoporometry technique** was implemented for **low-field** (using tert-butanol as test liquid) **and high-field** NMR instruments, and optimized for numerous porous materials (aerogels, clay minerals, cement-based binders, polymer gels). Using low-field instrument can enlarge the technical possibilities while decrease the expenses of these measurements.[1, 2, 4]
- **A model is under elaboration for such pore geometries where the cylindrical and spherical pore shape is not applicable** in the modified Gibbs-Thomson equation. In several cases the hysteresis of the measured freezing and melting curves is between the spherical and cylindrical model, thus *n* in equation 1 is between 2 and 3. On the basis of the measured data and theoretical considerations, a modified model is being formed.

$$\Delta T_{m/f} = T_{m/f} - T_0 = -\frac{nK_c}{r_p} \quad (1)$$

where $T_{m/f}$ is the melting and freezing point of the liquid in the porous system, T_0 is the transition temperature of the bulk liquid, n is a factor characteristic for the pore geometry, K_c is the cryoporometric constant of the liquid (determined by the V_m,molar volume, γ_{SL},solid-liquid interfacial tension, ΔH, heat of melting and the T_0 of the liquid), while r_p is the radius of the pore.

- In case of narrow pore size distributions even the **surface relaxivity** (ξ) can be derived as the pore shape and size is known from cryoporometry (Eq. 1 and 2.). Its exact value is very difficult to determine experimentally otherwise.[2]
- **Vapor and restricted diffusion** were observed in partially filled pore structures. This means a novel way for the detection of the complete saturation of mesopores, also supported by NMR relaxometry and cryoporometry.[2]
- **Self-diffusion coefficients of confined liquids** were determined on low- and high-field NMR instruments, using **spin-echo and Hahn-echo methods**. In the case of porous samples containing paramagnetic impurities (e.g., cement-based samples), **H_2O-D_2O exchange technique** was implemented, using the mathematical model describing the diffusion from cylinders.[3-5]
- **The effect of thermal convection on the time-dependence of diffusion constants** was detected and experimentally confirmed.[3]
- ***T_2* relaxometry** technique was used for **the characterization of hydrophilic and hydrophobic surfaces**. Through the T_2 relaxation time constants of polar and non-polar liquids confined in porous materials, information was gained on the hydrophilic/hydrophobic properties of the pore surface. Furthermore, the affinity of the surface toward polar/nonpolar adsorbates can be predicted which is

important for numerous potential applications (like industrial catalysts and environmental adsorbents).[1, 2]

- **The evaluation of T_2 exponential curves is already routinary** with inverse-Laplace transformation (especially for rocks with several relaxation domains) and by exponential fitting with the least-square method.
- ***T_2* relaxation time constants measured in time** were used for the description of any kind of processes, where the pore size or the surface properties change as a function of time, e.g., curing processes and rehydration of silica-based binders, swelling kinetics of polymer gels. [4]
- Information gained from NMR relaxometry data was broadened with the **temperature depending measurement of *T_2* relaxation time constants**. The change of the quantitative value of the test liquid during phase transition refers clearly to the pore size, while the change of the T_2 time constants bear extra information about surface properties.
- ***T_2* relaxation time constants** measured during the saturation of the pore system was applied for determining the **filling mechanism of the pores**, and drawing conclusions about the **pore size and its polydispersity.** The application of a *k* factor in the basic equation of the T_2 relaxivity, gives information about the distribution of the liquid during the saturation of the pores: fitting the T_2 values as a function of the filling factor (*f*) gives a *k* close to 1 when the whole surface layer participates in the exchange process, while it is closer to zero when the filling process is plug-like. This model was successfully used in the case of the mesopore system of carbon aerogels. However, it was also concluded that in case of polydisperse pore system, the model is impossible to be used, as the measured T_2 value is dependent on the pore size and shape (the surface, *S* and the volume, *V* of the pores). See equation 2.[2, 4]

$$\frac{1}{T_2} = \xi \frac{S}{V_0} \frac{1}{f^k} + \frac{1}{T_{2b}} \qquad (2)$$

- ***T_1-T_2* correlation measurements**, which is often used in the characterization of rocks and describes the connection of different relaxation domains, were implemented to our instruments by Dávid Nyul PhD student (under shared supervision) and tested for several systems.
- **The NMR Mobile Universal Surface Explorer (MOUSE)** was successfully applied for the surface characterization and mapping of siltstone boreholes. Due to different relaxation properties, the compounds of the borehole can be distinguished on the surface or even in 5 mm depth.
- **Complex use of NMR relaxometry, cryoporometry and diffusometry:** Application of various NMR methods combined with sorption techniques can reveal such differences between porous materials which remain hidden at separate use of the techniques. The N_2 gas adsorption method gives information about the dry structure of the synthesized aerogels, XPS describes the chemical composition of the surface while water vapor adsorption, beyond the surface chemistry, points at the behavior in wet state, that is under the circumstances of possible applications. However, the combined use of NMR relaxometry, diffusometry and cryoporometry is able to provide a complex

description and model of the hydration and pore filling mechanism of porous materials up to the oversaturated state. The joint use of low- and high-field NMR instruments support the characterization in a unique way.[2]

Collaborations and further results:

- I am in contact for several years with ***Prof. Dr. Krisztina László (Budapest University of Technology and Economics)***, and this collaboration was continued in the past three years. I carried out NMR measurements detailed above on carbon-based materials, several of which were synthesized in her research group, while she helped us with the pyrolysis of polymer aerogels and gas porosimetry data. The valuable discussions with her about the properties of carbonaceous materials supported the published two papers in this topic.
- A long-term cooperation was started with the ***Isotoptech Zrt.*** in 2021, in the framework of which metakaolin modified cement composites and other silica-based binders, like geopolymers are synthesized, and characterized, according to the standpoints and requirements of the ***Public Limited Company for Radioactive Waste Disposal***. The above-mentioned results on these porous materials have high importance in the long-term modelling of radioactive waste disposal and in the management of special radioactive wastes, like ion exchange resins and acidic wastes. Discussions were made about further NMR experiments on siltstone borehole samples as potential reservoir rocks for the long-term storage of high-level activity uranium rods.
- Scanning Electron Microscope (SEM) images were taken and XPS measurements were executed on various carbon aerogels and metakaolin modified cements in the ***Institute for Nuclear Research by Attila Csík and Tamás Fodor***.
- I initiated an international professional connection with ***Prof. Ioan Ardelean***, the head of NMR diffusiometry and relaxometry laboratory at the ***Technical University of Cluj Napoca***, Romania. After two personal discussions about collective work of porous materials with their Fast Field Cycling NMR relaxometer me and my PhD student Vanda Papp are travelling to Cluj Napoca for FFC relaxometry measurements on metakaolin-modified cement and carbon aerogel samples this October.
- In the third year of the project, Small Angle Neutron Scattering (SANS) measurements were carried out on metakaolin-modified cements in the ***Budapest Neutron Centre*** with the help of ***Adél Len***. Vanda Papp PhD student under my supervision, fitted the gained scattering curves with novel modelling methods in a collaboration with ***Cedric J. Gommes (School of Engineering, University of Liège, Liège, Belgium)***. These results, supported with our NMR relaxometry data lead to a more-detailed model for the exact structure of these binders and the effect of metakaolin on the cement morphology, and are summarized in a manuscript under preparation.

- The above-mentioned NMR methods were applied in the characterization of swelling cross-linked biodegradable polymers synthesized by the research group of ***Prof. Sándor Kéki (Dep. of Applied Chemistry, University of Debrecen)***. The kinetics of swelling in different liquids was followed and the mechanism was described on the basis of T_2 relaxation data. The publication is before submission (**V. Papp, B. Vadkerti, S. Kéki, I. Bányai, M. Kéri*, Swelling properties and structure of biodegradable crosslinked polyurethanes by NMR**).
- As a preliminary work towards to ionic liquid containing porous supercapacitors, I carried out conductivity measurements on acetic acid – methyl-imidazole mixtures in a collaboration with ***Prof. Dr. Barbara Kirchner (Mulliken Center for Theoretical Chemistry, University of Bonn)*** and colleagues from our department (Dep. of Phys. Chem., UD). The contribution to their theoretical results with experimental data resulted in a high-impact publication.[6] This collaboration is intended to be continued with high-field NMR study of ionic liquid systems.
- I applied my NMR experience (1D, 2D NMR, diffusion studies) in a collaboration with colleagues from our department, through the NMR description of complexing properties of small molecular ligands with rare earth metal ions. As a result, one scientific paper was published in 2022 [5] and a second one is under review after a revision in Dalton Transactions **(Sz. Bunda, N. Lihi, Zs. Szaniszló, D. Esteban-Gómez, C. Platas-Iglesias, M. Kéri, G. Papp and F. K. Kálmán: Bipyridil-based chelator for Gd(III) complexation: kinetic, structural and relaxation properties, Dalton Transactions, RSC, 2023, IF: 4.57, Q1, under review)**.
- Recently, preliminary experiments were carried out in a collaboration with the ***University of Szeged (Edit Csapó and Ádám Juhász)*** on the NMR diffusion measurements of polymer-surfactant systems.

Others:

Thanks to the frequent participation of our research group on the Alpine NMR Workshop in the previous years with NMR results on confined liquids, we had the pleasure to organize the conference in Hungary in 2023. It took place in Mátrafüred between 14-17. September 2023 with the presence of colleagues from Slovenia, Germany and Romania.

Outlook:

The results detailed above form the basis of several publications and further researches in the future. Carbon-based porous materials are in the focus of researches as potential supercapacitors and battery materials. For these applications the basic knowledge of diffusion and behavior of ionic solutions and ionic liquids is essential, thus the presented results and NMR methods are planned to be used for this purpose. Metakaolin as potential additive and geopolymer compound is to be further studied due to the increasing demand on the conditioning of special radioactive wastes in the future. NMR MOUSE seems

to be unique in the surface mapping of monolith samples, thus efforts will be made for the study of rock composition, soil structure, evaporation processes. Correlation experiments could give extra information on the exchange processes of different water domains in porous solids, for this reason T_2-T_2, T_2-diffusion experiments are planned to be implemented on our instrument, and applied for several types of materials.

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[1] M. Keri, B. Nagy, K. László, I. Bányai, Structural Changes in Resorcinol Formaldehyde Aerogel seen by NMR, Microporous and Mesoporous Materials 317 (2021) 110988.

[2] M. Kéri, D. Nyul, K. László, L. Novák, I. Bányai, Interaction of resorcinol-formaldehyde carbon aerogels with water: A comprehensive NMR study, Carbon 189 (2022) 57-70.

[3] D. Nyul, L. Novák, M. Kéri, I. Bányai, A Simple Elimination of the Thermal Convection Effect in NMR Diffusiometry Experiments, Molecules 27(19) (2022).

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[6] L. Wylie, M. Kéri, A. Udvardy, O. Hollóczki, B. Kirchner, On the Rich Chemistry of Pseudo-Protic Ionic Liquid Electrolytes, ChemSusChem 16 1-14 e202300535.