Fast Laplace NMR methods for time-dependent processes analysis

Nuclear Magnetic Resonance (NMR) spectroscopy is one of the most versatile analytic tool known to mankind. Since its dawn in the late 1940s, it has become successfully implemented as a research tool in many areas like: organic chemistry, food and drug control, biological research and even in the form of Magnetic Resonance Imaging (MRI) in the medical diagnostic.

One of the unique analytical application of NMR is the study of heterogeneous materials like, e.g. sandstone or rubber. Such materials have crucial importance in modern word. For example, sandstone in many parts of the world is a reservoir of the oil deposits. For such materials the special branch of NMR have emerged: Laplace NMR (LNMR). The LNMR technique relies mainly on the measurement of three phenomenons: Longitudinal relaxation, transverse relaxation and diffusion. The first two parameters describe how the nuclear magnetic spin is returning to equilibrium, and the last describes how fast the molecule is being transported. Those parameters are incredibly sensitive to the environment and allow to study many different materials.

To further enhance the capabilities of LNMR, one can measure two-dimensional correlation maps between relaxations and diffusion coefficient. Such maps provide much richer information but in the cost of time. Each point of the second dimension (called indirect) is recorded by repeating the whole measurement. Therefore 2D LNMR may require even hours to acquire single correlation map. This feature blocks the technique usage for fast-changing systems like reactions.

The aim of this project is to enable usage of 2D LNMR for reaction monitoring and time-dependent processes analysis by circumventing the long acquisition time limitation. The project will use two novel techniques that will allow monitoring changes in the measured systems:

1. Ultra-fast Laplace NMR (UF-LNMR)
2. Time-resolved Laplace NMR (TR-LNMR)

First technique, instead of repeating the measurement for each indirect point, will encode the indirect dimension along the sample. So each part of the sample corresponds to a different point of the second dimension. Such approach allows measuring the 2D experiment in the time of 1D. Therefore UF-LNMR allows studying fast processes by repeating the experiment for different moments of the process.

The second technique, also known as moving-frame, relies on the repetition of the experiment many times (during the process study) with different random values of indirect dimension stop. After the acquisition, the set of the experiments is divide into small frames that overlap. Each frame corresponds to single-time value of the process and as the frames are overlapping, the time difference between those is minimal. That allows regaining the temporal resolution non-achievable with the classic approach.

The combination of those two methods will allow studying many time-dependent processes with 2D LNMR techniques, which was not achievable before. To popularize the technique among scientific community, the software package for acquisition, processing and analysis of the new methods will be developed.

The method will be utilized mainly to understand the mechanism of important for industry processes like hydrogenation or polymerization. Appart from that, fast LNMR methods will be used to study other time-dependent processes, like: food production, absorption processes, reactions in ionic liquids, polymer studies on polymerization and degradation.