

Novel insight into complex reactions. A portable setup for Time-resolved Non-uniform sampling and Laplace NMR

Nuclear Magnetic Resonance (NMR) spectroscopy is one of humankind's most versatile analytic tools. Since its dawn in the late 1940s, it has been 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 medical diagnostics.

One of the unique analytical applications of NMR is the study of complex reactions. The reaction monitoring capabilities allow us to study the change in the concentration of reactants over time. Recently, we have presented a new way of analyzing the complex polymerization processes using a combination of two independent NMR techniques: Time-resolved Non-Uniform-Sampling and Time-resolved Diffusion NMR. The first technique allows one to follow the concentration changes of molecules in the reaction mixture. At the same time the second gives us information about the changes in the mobility of reactants and their molecular mass. The combination of both methods resulted in a new, more profound understanding of the polymerization process and a much more complex insight into the reaction mechanism.

In this project, we plan to enhance the capability of the new method and increase its applicability. We intend to adapt it to the cheap, portable low-field spectrometers to be able to follow complex chemical reactions carried out in standard laboratory flasks and reactors instead of being limited to the simple reactions inside the NMR tube.

We want to test the new, freshly developed setup on two classes of polymerization. Photopolymerization is a growing field in material science and is gaining immense importance as biocompatible 3D printing is utilizing this methodology. The second class is click-chemistry-based polymerization, based on the simple and elegant methodology proposed by the 2022 Nobel Laureates in Chemistry Bertozzi, Meldal, and Sharpless.

The last goal of the project is to combine the newly developed methodology with automation and machine learning to create an automatic setup for optimizing the reactions mentioned above. This new setup will allow us to completely control the reaction and achieve the desired length of polymers with good yields.