Project 3.1 Synergy of Time Resolved Non Uniform Sampling and Diffusion NMR for Automatic Reaction Optimization

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Background:

Nuclear Magnetic Resonance (NMR) spectroscopy is one of the most versatile analytic tools. One of the unique analytical applications of NMR is the study of 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 and click-reactions.

The last goal of the project is to utilize the newly developed methodology to create an automatic setup for optimizing the reactions mentioned above.

Aim:

The project aims to create a new setup for studying complex polymerization reactions using a low-field NMR spectrometer.

Requirements:

- M.Sc. in Chemistry, Physics, or similar,
- basic knowledge of NMR,
- hands-on laboratory experience