Project 3.7 Application of fast Laplace NMR methods for reaction monitoring

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Background:

Laplace NMR methods have been widely used for many years in industry as well as in scientific research. This technology is based on the use of phenomena of longitudinal and transverse relaxation of atomic nuclei and diffusion to study processes in both homo and heterogeneous materials. Thanks to its independence from chemical shift (in contrast to classical NMR), it allows not only to study materials with very different structures (e.g., concrete, rocks, polymers, food, tissues) but also enables the use of simple NMR analyzers, which do not have a homogeneous magnetic field. This makes it possible to significantly reduce the cost of measurement as well as the mobility of such devices (e.g., in the petrochemical industry, such devices are used in well logging). Until now, the main limitation for these methods has been the measurement time for multidimensional techniques, which has significantly limited the application of Laplace NMR in the study of time-dependent processes. However, two fast methods based on this technique have recently been developed:

1.Ultra-Fast Laplace NMR

2.Time-resolved Laplace NMR

These techniques made it possible for the first time to study fast processes using multidimensional Laplace NMR with time resolution measured in seconds rather than tens of minutes, or even hours. As these techniques are relatively new they have so far mainly been used in simple demonstration systems rather than for studying reactions.

Aim:

In the project we will use fast Laplace NMR techniques to study important time-dependent processes. The research will focus on 3 topics:

1. hydrogenation reactions using para-hydrogen (hyperpolarization by PHiP and SABRE)
2. photopolymerization
3. production of dairy products.

These phenomena will be studied on both high and low field NMR spectrometers. The project will be carried out in collaboration with the University of Oulu (Finland) as well as the Institute of Innovation of Dairy Industry.

Requirements:

- M.Sc. in chemistry, physics, biology, pharmacy, food engineering, material engineering or similar,
- basic experience with programming (preferably Python and/or Matlab) or willingess to learn,
- basic understanding of NMR is a plus,
- hands-on laboratory experience