Hyperpolarized parahydrogen based MRI: SLIC-SABRE and catalytic reactors imaging

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In Situ MRI of Heterogeneous Catalytic Hydrogenation with and without Hyperpolarization: Magnetic resonance imaging (MRI) is a powerful technique to characterize reactors in situ. However, low spin density for gas phase reactions and magnetic field inhomogeneity caused by the presence of a solid catalyst are challenging for MRI. Parahydrogen (p-H_2) induced polarization (PHIP) can significantly increase NMR signal. Here, we present a new type of catalytic reactors for MRI that allows to visualize distribution of gas flow utilizing PHIP, but also suitable for imaging of thermally polarized gases. MRI study of propene hydrogenation was done using FLASH (fast low angle shot) pulse sequence [1]. The stack of 2D slices obtained by MRI was transformed into 3D model (Fig. 1). However, catalyst is non-uniformly located on the reactors surface. Products formation occurs only near catalytically active regions. Therefore, MRI can be used for the characterization of the reactors structure. In addition, reactions of 1,3-butadiene and propyne hydrogenation were investigated. The 1D maps of reagents and products distribution along the system were imaged using spin-echo pulse sequence. In conclusion, the structure of the reactors and compounds distribution along the system were obtained due to the high stability and the fabrication simplicity of the reactors.

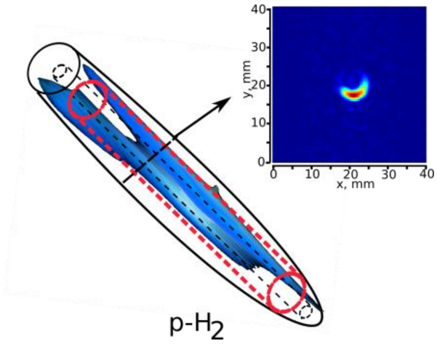

Fig. 1: 3D model of the gas flow. The black solid line shows the edges of the NMR tube, the red dashed line - the reactor, the black dashed line - the capillary.

^{15}N MRI of ^{15}N-labelled and non-labelled biomolecules using SLIC-SABRE: Signal amplification by reversible exchange (SABRE) is another hyperpolarization method based on p-H_2. It allows to obtain hyperpolarized substrate without any structural transformation. The use of ^{15}N nuclei for imaging can extend the application of MRI in biomedicine because of no background signal from ^{1}H nuclei during in vivo studies and longer T_1. For polarization transfer from ^{1}H to ^{15}N we used SLIC-SABRE pulse sequence. ^{15}N MRI of ^{15}N-pyridine (^{15}N-Py), ^{15}N-nicotinamide (^{15}N-NA, vitamin B_3), 4-aminopyridine (fampridine) and dimethylaminopyridine (DMAP) was done using single point imaging (SPI) or FLASH. It should be noted that fampridine is a drug, which cures the symptoms of multiple sclerosis. We compared the effectiveness of two imaging pulse sequences utilizing ^{15}N-Py and ^{15}N-NA [2]. FLASH pulse sequence provides the shorter imaging time, while SPI provides the higher spatial resolution. However, for the future applications, it is better to decrease imaging time, therefore, FLASH pulse sequence was chosen for MRI of non-labelled compounds (Fig. 2). The high level of ^{15}N polarization (≈8 %) allowed to do ^{15}N MRI of biomolecules with natural abundance of ^{15}N for the first time.

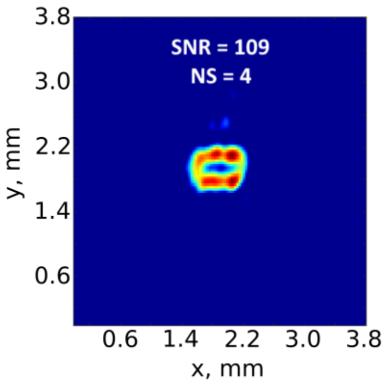

Fig. 2: ^{15}N FLASH MRI of fampridine. The void in the center corresponds to the presence of the capillary supplying p-H_2.

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References: [1] Kovtunov et al., ChemCatChem (2018). [2] Svyatova et al., Chem. Eur. J. (2019).