Operando MRI study of a heterogeneous reactor using parahydrogen-induced polarization with antiphase-to-inphase signal shape conversion

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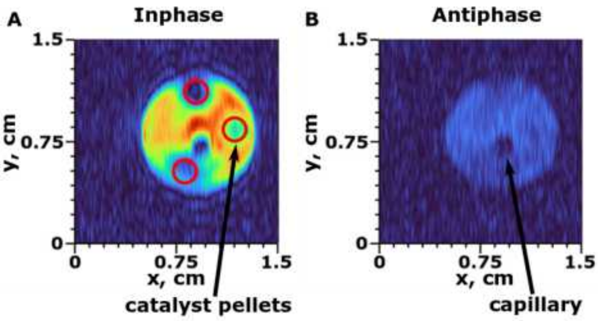
Magnetic resonance imaging (MRI) methods can be used for operando studies of heterogeneous catalytic processes in the gas phase. As the spatial distribution of reactants and reaction products is not uniform, MRI allows one to get a more detailed understanding of the heterogeneous reactor operation. However, there are many factors, including low spin density, magnetic field inhomogeneities, fast diffusion and short relaxation times of gases, which complicate such studies and make it essential to use hyperpolarization. Spin hyperpolarization techniques in general, and parahydrogen-induced polarization (PHIP) in particular, provide a major increase in the intensity of NMR signals. At the same time, an antiphase lineshape of NMR signals associated with PHIP at high magnetic fields is disadvantageous for MRI experiments because it leads to mutual cancelation of the positive and negative parts of such signals [1].

Results of this work demonstrate the importance of antiphase-to-inphase signal shape conversion in MRI experiments to utilize the signal enhancement provided by hyperpolarization to the maximum possible extent. This approach, implemented for the first time in an MRI study of an operating model reactor, allowed us to achieve a 10-fold improvement in signal-to-noise ratio compared to the usual experiment performed on an antiphase signal. This made it possible to visualize catalyst beads in the 3D MR image obtained (Fig. 1 A).



hyperpolarized propane in a model reactor obtained with (A) and without (B) conversion of an antiphase signal to an inphase one.

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[1] D.A. Barskiy et al., *J. Phys. Chem. C.* **2017**, *121*, pp. 10038-10046.