Chemically Resolved MRI with Field Inhomogeneity Correction

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Introduction: Magnetic Resonance Imaging (MRI) allows spatially resolved *in situ* identification of chemical species via their shifts from the proton resonance frequency, which is beneficial in chemical engineering. However, traditional spectroscopic methods are time-consuming at high spatial resolutions. Recent techniques adapt non-spectroscopic sequences by incorporating prior knowledge of chemical species spectra to overcome this constraint [1], but they remain sensitive to magnetic field inhomogeneities, particularly in large-bore systems. This work addresses that limitation by combining field inhomogeneity correction with chemical species reconstruction in a unified method.

Methods: We extend the forward model by Harbou *et al.* [1], which combines weighted *k*-space contributions from individual chemical species based on their spectra, introducing both amplitude scaling and phase shifts. The model represents a superposition of the Fourier transform and a chemical shift operator. Here, we further modify the Fourier operator to incorporate field inhomogeneity maps [2], enabling the model to account for spatial phase variations. Experiments were conducted on a cylindrical water phantom with an inserted tube containing acetone–water mixtures at varying ratios. Data were acquired using a multi-echo gradient echo (mGRE) sequence with 32 equidistant echoes (1.81 ms spacing, starting at 1.1 ms), yielding a 21.5 s scan time for a 16 cm × 16 cm field of view and an 80 × 80 grid.

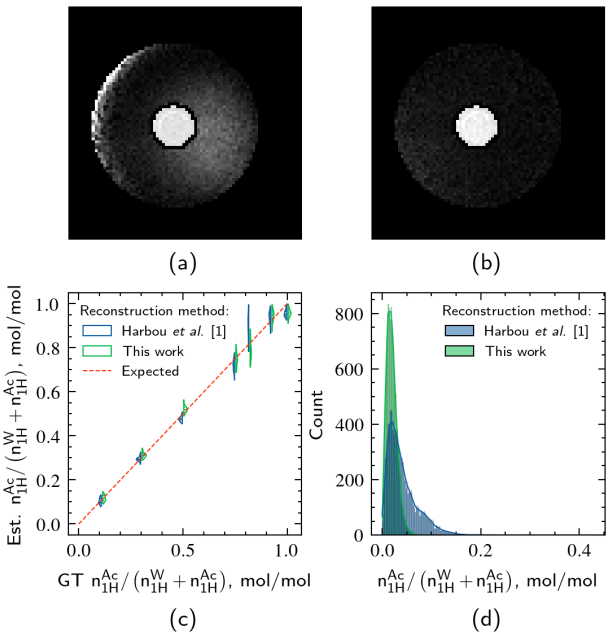

Fig. 1: Chemically resolved reconstruction in the transverse plane of a tube with an acetone–water mixture submerged in a larger tube: (a, b) acetone ratio maps with (a) and without (b) field inhomogeneity correction; (c) acetone ratio distributions in the inner tube across varying concentrations; (d) ratio distribution in the outer tube across experiments.

Results and Discussion: Fig. 1(a–b) shows reconstructions for an acetone proton molar ratio of 0.3 in the inner tube, with and without field inhomogeneity correction. Artifacts–visible as white regions in the outer tube–are removed after correction, yielding a more homogeneous appearance. Image quality in the inner tube remains unchanged. Fig. 1(c) shows acetone ratio distributions in the inner tube. The mean absolute errors (MAEs) are 0.033 ± 0.024 (with correction) and 0.026 ± 0.013 (without), with no significant difference (Wilcoxon signed-rank test: $p = 0.375$, $n = 7$). In the outer tube (Fig. 1(d)), the MAEs are 0.041 ± 0.012 and 0.020 ± 0.002, showing a significant improvement after correction ($p = 0.016$, $n = 7$, $\alpha = 0.05$).

Conclusion: This work presents a reconstruction method that simultaneously resolves chemical species and corrects field inhomogeneity artifacts in non-spectroscopic Cartesian mGRE data. It achieves ~3% precision in estimating the acetone–water ratio. Correction effects are most evident in the larger water-filled region—an important consideration, as real-world samples are often similarly sized. Future work should focus on designing experiments that better reveal the expected effects in the smaller mixed region, where differences may have been masked by its limited size.

References: [1] Harbou, J. Magn. Reson. (2015). [2] Eggers, IEEE Trans Med Imaging. (2007).