Quantitative T₁ Imaging for Battery Characterisation

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Introduction: Current lithium-ion batteries have problems with sustainability and safety [1], hence new battery technologies are being sought which can address these issues. As a consequence, new electrodes and electrolytes are being developed. However, in addition to new materials, new characterisation techniques are also required that enable *in situ*, real time monitoring of chemical processes across the electrode and electrolyte. Nuclear magnetic resonance (NMR) methodologies offer non-invasive characterisation of the chemical compositions of such materials, which can then be spatially-resolved using magnetic resonance imaging (MRI) [2,3]. Using MRI, we have been investigating novel ionic liquid (IL) battery electrolytes. By using the NMR relaxation time of the IL, we are able to map the distribution of chemical species within the IL enabling *in situ* visualisation of battery chemistry [4]. However, the variation in relaxation times can sometimes be small and, therefore, it is important to maximise the signal-to-noise ratio (SNR) to reduce the T_1 standard deviation (σ) and enable quantitative and accurate determination of relaxation times. A systematic study has been undertaken to investigate and optimise the influence of experiment type, signal averaging, and echo summation on the SNR. These techniques have been employed to quantitatively map the composition of ILs for novel battery applications.

<u>Methods</u>: ¹H and ¹⁹F MRI T_1 maps of a series of CuSO₄ concentrations and an IL respectively were acquired using a RARE pulse sequence with either saturation recovery or inversion recovery methods, and analysed by summing the echo images or using the first echo image. The average T_1 and σ values were determined for each different solution as a function of experimental parameters.

Results and Discussion: By comparing the T_1 maps for a series of CuSO₄ concentrations, it was demonstrated that inversion recovery resulted in a lower σ than saturation recovery. As expected, signal averaging improves the SNR, and decreases the σ , but increases the experiment time. However, by summing multiple echoes it was possible to increase the SNR, and decrease the σ , without increasing the experiment time. When the optimised methodology was applied to observe the absorption of water in an IL, the change in T_1 became observable on a timescale sufficiently rapid to detect the ingress of water.

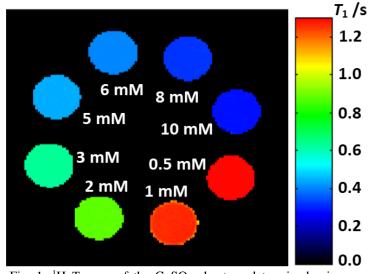


Fig. 1: ¹H T_1 map of the CuSO₄ phantom determined using an inversion recovery experiment.

Conclusion: A systematic study exploring methods for reducing noise in T_1 maps has been performed. It was found that the SNR can be improved, and the standard deviation decreased, by increasing signal averages. However, this comes at a cost of increased experimental time. An alternative method was to sum the echo images, which does not result in an increase in experimental time.

References: [1] Grey, Nat. Matter. 16 (2016) 45. [2] Britton, Chemphyschem, 15 (2014) 1731. [3] Bray, Angew. Chem. Int. Ed. Engl. 55 (2016) 9394. [4] Britton, J. Phys. Chem. Lett. 4 (2013) 3019.