



Nanoscale Organisation
and Dynamics Group

Extracting Information from NMR Spectra of Coal

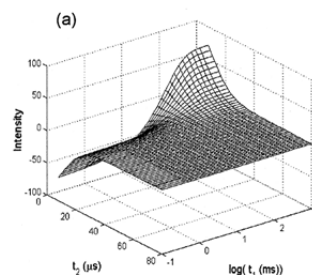
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Marcel Maeder

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Abstract

The ideal situation for the NMR spectroscopist is a homogeneous solution of one component and a high field NMR instrument. Possibly the worst situation is a solid mixture of an 'infinite' number of different components and a low field NMR instrument: e.g. NMR spectroscopy of black coal powders on a 20MHz instrument. Our method to characterise this material in terms of parameters useful for industry is based on a robust and extensive quantitative determination of different relaxation processes. This can be described as measuring T_1/T_2 decay surfaces, followed by a least-squares analysis based on different models.

The project goal was to investigate the possibility of methods that could support or replace traditional coal analysis methods which can be slow and expensive. To achieve this the PLS (partial least squares) method was developed to relate the least-squares analysis results to known coal properties using extensive calibration. The results of the PLS calibration allow the prediction of coal properties solely based on the NMR response surfaced. The quality of the analyses results are astonishing.



Profile

Jeffrey Harmer is the Electron Paramagnetic Resonance (EPR) group leader at the Centre for Advanced Imaging, University of Queensland. His main research tool is Continuous Wave (CW) and pulse EPR which he applies to a wide range of problems with an emphasis on applications in structural biology and understanding the reactivity of metal complexes in chemistry and biology.

Marcel Maeder is a retired academic from the University of Newcastle. Originally a coordination chemist, Marcel has been active in chemometrics for a long time. Presently, Marcel is involved in a different aspect of coal, investigating the chemistry of CO₂ in aqueous amine solutions relevant for post-combustion capture.

Staff and students at all levels are welcome to attend.

Venue and Time: This talk will be held on 27th April at 2pm at the Campbelltown Campus in Building 21, Lecture Theatre 6 (CA.21.G.18).

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