

from the basic DOSY experiment can be enhanced by advanced, e.g. multivariate and multi-way processing and extended by incorporating information from other sources such as relaxation.

NMR spectra of mixtures are often very crowded due to the abundance of signals with multiplet structure caused by scalar coupling. In  $^1\text{H}$  NMR, multiplets caused by homonuclear scalar coupling are often many times the width of a single line, making it very difficult to distinguish individual chemical shifts in crowded spectra. An efficient method to collapse the multiplet structure has long been sought, but only recently have experimental methods for such homonuclear broadband decoupling become practical. These “pure shift” or “chemical-shift resolved” methods give resolution improvements approaching an order of magnitude, far in excess of any gains realistically to be expected from increases in static magnetic field.

### **The quality of soil organic matter, accessed by $^{13}\text{C}$ Solid State NMR, is more important than its content concerning pesticide adsorption**

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The need for food will increase by 59–98% from 2005 to 2050, and its global growth production has been achieved mainly through the intensive use of inputs such as pesticides and chemical fertilizers. Once released to the soil, sorption (represented by  $K_d$  values) and degradation are two governing processes that determine the distribution and persistence of pesticides.

In spite of the huge dataset, the only apparent generalization is the high correlation between  $K_d$  and soil organic matter (SOM) content. This is because the SOM is the main adsorption site for pesticides. Seeking to normalize the experimental data and to access the pesticides mobility, the  $K_{oc}$  value is calculated:  $K_d$  normalized by soil organic C content (C).

However, in this work no correlation was observed between  $K_d$  and C and so the obtained  $K_{oc}$  spread out in a wide range: 1,100 to 11,400  $\text{mL g}^{-1}$  for Abamectin; and 30 to 150  $\text{mL g}^{-1}$  for Atrazine, both ranges corroborate with data from literature. These high variability indicate that something else strongly interfere in the pesticide sorption as just the SOM content. The Principal Component Analysis of the  $^{13}\text{C}$  NMR spectra of the soil humic acids, a fraction of the SOM, generated the first PC with negative loads for the aliphatic compounds and positive for the aryl C, typical of partially oxidized pyrogenic C.

Their scores showed strong correlation with the Abamectin  $K_{oc}$  values ( $R^2=0.91$ ) and weaker with Atrazine  $K_{oc}$  ( $R^2=0.60$ ,  $p<0.0001$ ), besides with a smaller standardized slope: 1.01 for Abamectin and 0.76 for Atrazine. These results could be explained by the higher hydrophobicity of Abamectin, being thus more prone to interact with the polycondensed aryl groups from the pyrogenic C.

Another point that must be stressed is that humic acids are useful proxy to understand the interaction of the SOM with pesticides.

### **Optimising diffusion editing measurements in borehole magnetic resonance towards adsorbed gas quantification**

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Determining gas content in coals is fundamental for commercial mining operations. Recent developments in coal seam gas (CSG) exploration and production has generated considerable interest in providing accurate *in-situ* gas quantification. Gas content in coal seams is currently determined using core cannister desorption measurements which involve a time-consuming laboratory core evaluation and are problematic due to gas lost in the core recovery process as well. Therefore, an opportunity exists for developing a rapid and accurate measurement procedure for gas quantification in CSG.

We present a novel technique for measuring gas concentrations using borehole magnetic resonance (BMR). Multi-dimensional diffusion editing sequences have previously been used to quantify fluid volumes in conventional oil and gas reservoirs. In CSG, fluid can exist as free gas or adsorbed gas; which is a liquid-like membrane adhered to the coal interface. Adsorbed gas exhibits a different magnetic resonance response relative to free gas and oil. The diffusion-editing pulse sequence must be appropriately designed to ensure sensitivity to the fluid volumes of interest. We demonstrate how the diffusion timing parameters can be optimised towards measuring free and adsorbed gas. The optimised diffusion-editing sequence is used to capture BMR measurements of coal seams. The measured data is inverted using a 2D