Invited Abstracts

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I-01

PROBING DIFFUSION ON, OF AND IN SPHERES

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Magnetic Resonance measurements of diffusion are able to probe the shape and size of structures too small to be directly visualised using MRI. These measurements are also able to investigate transport, exchange and dynamics. In systems where diffusing molecules are confined to the surface of a sphere, the probability distribution function for molecular displacement (*P*(*D*)) changes from a Gaussian function, which is typically observed for molecules diffusing in bulk, to a propagator with a 'cusp-like' shape at zero displacement[1]. By measuring the propagators for molecules diffusing in or on a sphere surface, it is possible to confirm the location and geometry of region in which these molecules reside, as well as determine their mobility. Equally, measurements of diffusion for molecules comprising the spherical structure can also provide information about the size and mobility of that structure[2], as well as its composition.

In this talk, I will present three studies which have employed diffusion measurements to probe molecules which are either moving in or on the surface of spherical structures or form the spherical structures themselves. These spherical structures are reverse micelles in a microemulsion, the pores in a foam and prilled urea. In all of these systems, the variation of observation time becomes a powerful tool for studying the size and shape of the composite structures, as well as the dynamics of each system.

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I-02

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The aim of this presentation is twofold: Firstly, to explore the potential of simultaneously acquiring multimodal MR-PET-EEG data in a human 9.4T scanner to provide a platform for metabolic brain imaging. Secondly, to demonstrate that the three modalities are complementary, with MRI providing excellent structural and functional imaging, PET providing quantitative molecular imaging, and EEG providing superior temporal resolution. A 9.4T MRI scanner equipped with a PET insert and a commercially available EEG device were used to acquire *in vivo* proton-based images, spectra, and sodium- and oxygen-based images with MRI; EEG signals from a human subject in a static 9.4T magnetic field; and demonstrate hybrid MR-PET capability in a rat model. High-resolution images of the *in vivo* human brain with an isotropic resolution of 0.5mm and post mortem brain images of the cerebellum with an isotropic resolution of 320µm will be presented. A ^{1}H spectrum was also acquired from 2x2x2mm voxel in the brain allowing 12 metabolites to be identified. Imaging based on sodium and oxygen will be demonstrated with isotropic resolutions of 2mm and 5mm, respectively. Preliminary data from auditory evoked potentials measured in a static field of 9.4T will also be shown. Finally, hybrid MR-PET capability at 9.4T in the human scanner will be demonstrated in a rat model. Initial progress on the road to 9.4 T multimodal MR-PET-EEG will be illustrated. Ultra-high resolution structural imaging, high-resolution images of the sodium distribution and proof-of-principle ^{17}O data will be presented. Further, simultaneous MR-PET data without artifacts and EEG data acquired at 9.4 T will be shown.

I-03

PETROPHYSICAL APPLICATIONS OF NMR : TOOLS FOR UNDERSTANDING TRANSPORT IN POROUS ROCK MATERIALS

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During the last decades, NMR technology has found widespread applications in hydrocarbon exploration and production technologies. The NMR methods traditionally involved in this approach include NMR logging, which relies on lowering probes into the wellbore for measuring the NMR response of hydrocarbons several thousands of meters below surface, and low-field NMR relaxometry carried out in the laboratory setting with the goal to calibrate logging tools and to reduce the uncertainty in the interpretation of NMR logging data. More recently, the set of applicable methods has been augmented by MRI applications, which are used to quantify the distribution of the brine and hydrocarbon phases in core samples during experiments that test the feasibility and potential benefits of particular hydrocarbon recovery mechanisms. Furthermore, the development of NMR-based flow meters promises to make a step-change in the availability of accurate and cost-effective 3-phase flow meters that can be installed at well heads for providing real-time information of flow rates and fluid fractions of the gas, oil and water, fractions that are often produced simultaneously.

The presentation will summarize the main concepts and associated hardware of NMR logging and demonstrate with examples, how low-field laboratory NMR can be used to reduce the uncertainty in the interpretation of NMR logging data. In addition, experimental results will be shown that illustrate the applications and challenges of utilizing Magnetic Resonance Imaging during core flooding experiments related to Enhanced Oil Recovery applications. The presentation concludes with the introduction of the measurement concepts and hardware implementations of an NMR-based 3-phase flow meter which was developed jointly with industry partners.

I-04

DESIGN AND IMPLEMENTATION OF NMR SYSTEMS FOR DOWNHOLE EXTREME CONDITIONS

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Abstract: This presentation will describe the design and implementation of nuclear magnetic resonance (NMR) systems for downhole extreme condition at the China University of Petroleum from 2005 up to now. The extreme condition means the environment with high temperature (up to 175 C) and high pressure (up to 10000 psi) in a well bore, and very restricted space for tool size. Meanwhile, the tool is moving

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when the measurement is preformed, the sample is outside of the probe with the low magnetic field and low SNR. NMR system in downhole extreme conditions is very different from the conventional ones, so that special considerations have to be taken for probe and control system. And, the noise reduction, data processing and interpretation are also very important. This paper focuses on the key issues of design and implementation of downhole NMR System, including the design of components of the NMR system and signal flow; the design and implementation of probe, monitoring and control system; noise reduction methods, the design and implementation of data acquisition and processing software. The NMR system we proposed and designed has been delivered to engineering and application stage. It has significantly enhanced high end instruments and technology for China petroleum industry.

I-05

BIOCHAR SURFACE PROPERTIES AS ASSESSED BY FAST FIELD CYCLING NMR RELAXOMETRY

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Biochar (biologically derived charcoal) is a carbonaceous material produced by pyrolysis of biomasses. It is applied to soils in order to improve fertility and mitigate greenhouse-gases emissions. In fact, biochar changes physical-chemical soil properties, thereby affecting soil fertility. In addition, such porous material is also resistant to chemical and biochemical degradation. For this reason, its use allows carbon sequestration in soils and consequent reduction of carbon dioxide to the atmosphere.

Here, dynamics of water at the liquid-solid interface of water saturated biochars is discussed. Results revealed that water dynamics is affected by the nature of biochar parent biomasses. Moreover, biochar chemical physical properties are affected by conditions for their production.

It was understood that water undergoes to an inner-sphere interaction mechanism with biochar surface through formation of weak unconventional hydrogen bonds.

Recognition of the interaction mechanisms between water and biochar is of paramount importance in order to understand why biochar soil amendments improve soil fertility and crop production.

I-06

ACCESS OF MOLECULAR MOBILITY UNDER THE INFLUENCE OF INNER SURFACES OF HIGH-TEC NANOPOROUS MATERIALS BY NMR

Frank Stallmach, Tobias Splith, Carsten Horch, Anne-Kristin Pusch

University Leipzig

Transport and storage of fluids in porous materials is a topic encountered in many branches of science and engineering [1]. Direct access to these properties can be provided by NMR relaxation and diffusion studies. Such investigations are especially valuable for characterization of modern high-tec nanoporous materials, if they are performed with the pore fluids which will be present in the desired application. Having the potential of nanoporous materials for gas storage and gas separation in mind, the required narrow pore size and the strong adsorbate-adsorbent interaction strongly effect relaxation times and diffusivities of valuable gas molecules. On the example of methane and carbon dioxide in the metal-organic frameworks (MOF) HKUST-1 and ZIF-8, in zeolite ZSM-58 and in a polymer-based spherically shaped activated carbon (PBSAC), we will demonstrate how ^{1}H and ^{13}C NMR may be used to characterize pore structure parameters and adsorption capacities of the nanoporous materials [2-4]. Corresponding NMR diffusion studies were be used to probe the connectivity and dimensionality of the pore space of the respective adsorbents. They also clearly indicate fundamentals of host-guest interactions like size selectivity of pore windows and provide in combination with molecular dynamic computer simulation a comprehensive picture on the transport mechanisms on a molecular level. The presentation introduces the experimental set-up for NMR diffusion and relaxation studies at elevated gas pressures which is a necessary precondition for such studies with adsorbed gases.

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[3] B.-T. L. Bleken, K. P. Lillerud, T. Splith, A.-K. Pusch, F. Stallmach, Microporous and Mesoporous Materials 182 (2013) 25–31

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I-07

COMPACT NMR SENSORS FOR ON-LINE MONITORING: APPLICATIONS IN INDUSTRY, CHEMISTRY, AND MEDICINE

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Compact nuclear magnetic resonance (NMR) is finding applications for on-line monitoring in several research fields. The versatility of these devices has made possible the integration of NMR in different production setups ranging from extrusion lines to chemical reactors. In most industrial processes the sample under study is in continuous movement through the magnet at the time the measurement needs to be performed. This is the case when the magnet is integrated in a production line, or when a reaction mixture is continuously pumped for real time sampling. In this work we will present different examples where imaging, flow imaging, or spectroscopy methods are implemented under these conditions. In particular, we will discuss the available approaches for high resolution NMR spectroscopy for different reactions setups. A second example involves MRI experiments for assessing velocity information within aneurismal models in the presence of metallic flow. In this case, different alternatives for a fast monitoring will be discussed. Finally, the performance of fast imaging methods for quality control of extruded polymers will be presented.

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I-08

Analytic theory of 2D NMR in systems with coupled macro and micro pores

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Two dimensional (2D) nuclear magnetic resonance (NMR) experiments involve a sequence of longitudinal (T_1) and transverse (T_2) measurements. When such experiments are applied to porous media, they are believed to provide new and important information regarding diffusive coupling between distinct pore sub-populations. However, we show in this Letter that, in many cases of interest, this is simply not true. One often encounters systems in which the one dimensional (1D) T_1 and T_2 processes are each controlled by just two distinct decay modes. If these modes form a complete set, then one can derive analytic formulae that describe, exactly, the 2D NMR measurements. Therefore, for such systems, the 2D measurements bring it *no additional information* over that which is already present in the 1D results. Our predictions agree quite well with numerical results based on the microporous grain-consolidation (μ) model.

I-09

STRATEGIES FOR THE ACQUISITION OF J-SPECTRA USING PARAHYDROGEN INDUCED POLARIZATION

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The application of parahydrogen for the generation of hyperpolarization has increased continuously during the last years. When the chemical reaction that deposits the parahydrogen atoms into the target molecule is carried out at the same field as the NMR experiment (PASADENA protocol [1]) an anti-phase signal is obtained, with a separation of the resonance lines of only a few Hz. This imposes a stringent limit to the required homogeneity of the magnetic field in order to avoid signal cancellation. In this work we show that the spectrum of the PHIP signal acquired with a Carr-Purcell-Meiboom-Gill (CPMG) sequence, referred to as J-Spectroscopy [2], not only presents an enhanced spectral resolution compared to standard the NMR-spectrum, but also avoids partial peak cancellation.

Experimental and numerical simulations concerning the hydrogenation of Hexene with parahydrogen in PASADENA conditions are presented. Acquisition with a digital filter is used to select a desired multiplet, namely a partial J-Spectra acquisition [3]. The performance of the method is tested on a thermally polarized sample is included showing that the corresponding partial J-Spectra are unaffected by large inhomogeneities in the polarizing magnetic field [4]. Additionally we show that the method has the potential to discriminate PHIP-induced signals from thermal-induced ones, rendering a parahydrogen discriminated-PHIP J-spectrum (PhD-PHIP)[5]. Finally, limitations and applicability of the method to obtain either spectral information of the sample or to monitor chemical reactions of vey diluted samples will be discussed.

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I-10

ADVANCES IN NMR HARDWARE TECHNOLOGIES

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While NMR methods continue to advance in performance and application there is at the same time an advancement of the underlying hardware and software technologies. Three hardware areas experiencing rapid development are cryogen free superconducting NMR magnets, Field Programmable Gate Array (FPGA) based spectrometers and switch-mode (class D) RF power amplifiers.

The looming shortage of liquid helium and the recent advancements in cryo-coolers has driven the development of superconducting NMR magnets that do not use any liquid cryogens. There are several challenges to building NMR systems based on these new magnets such as vibrations from cryo-coolers, the inability to use superconducting shims and the electricity demands. However, a few MRI systems have been now been successfully developed and high field, high resolution NMR spectroscopy is very close to becoming a reality.

The introduction of FPGA devices has transformed the digital world and the use of this technology in NMR spectrometers has become commonplace. The performance and capacity of the devices has continued to increase to the extent now that nearly an entire spectrometer can be built using a single device containing functionality such as wide band digital receivers, multi Giga-sample per second direct digital synthesizers and complete processor systems running full featured operating systems such as Linux.

New high speed, high power MOSFETs have paved the way to the development of compact, high efficiency RF amplifiers delivering hundreds of watts up to frequencies of 20MHz. These new amplifiers together with the new FPGA developments are the key to new compact, power efficient mobile NMR systems.