Welcome to the 18th ISMAR 2013/14th NMR Users Meeting!

I am very proud of your participation at this event, which is the most important magnetic resonance event in Brazil and Latin America in the last 27 years. The scientific development of the world strongly depends on this topic, and each participant is certainly contributing with science and technology to improve human life condition.

This meeting is organized including ten Plenary Lectures, four Parallel Sessions with more than 150 lectures and oral presentations, three Poster Sessions and exhibit booths of 17 companies. The event is financed by 24 industries and 7 Brazilian foment agencies. The Student Grants were financed by 13 companies, a very important contribution for this event, helping economically 37 students.

Several actions necessary for all participants are financed by the event, for the comfort of participants like the wireless Internet system, freely available in the whole event region and transportation to the meeting, which is free and arranged for all the event participants and accompanying people. The respective information on transportation and internet is part of this book.

In this event we also have two satellite meetings, the Vth Iberoamerican NMR Meeting (Friday afternoon) and the Biomedical Imaging Symposium (Wednesday afternoon). To see the programs and to participate at the satellite meetings, it is necessary to register for them at the event's secretary desk. We strongly encourage everyone to join!

The social activities will start with a Welcome Reception on Sunday after the opening, honor and prizes lectures. On Thursday evening we will have the Brazilian Night at the Fogo de Chão Brazilian Steak House, including dinner, music shows and dancing. We strongly encourage your participation at this party, which will be a special opportunity for fraternization for all participants. Free transportation will be provided by the Meeting Organization.

Rio de Janeiro is a nice city, with many attractive sites, including mountains, beaches, forests, parks and districts, restaurants, museums, shopping and show centers. Wednesday and Friday afternoon/evening the ISMAR2013/14th NMR Users Meeting is also offering some excursions to the major touristic sites.

I hope you will enjoy this event and Rio de Janeiro!

José Daniel Figueroa-Villar
Chairman
18th ISMAR 2013/14th NMR Users Meeting

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fat content in commercial mayonnaises in sealed flasks. The analyses were performed using a CPMG sequence in a Spinlock (Cordoba, Argentine) TD-NMR spectrometer based on 0.23T Halbach magnet with 10 cm free bore. The comparisons between univariate model using the discrete values of transverse relaxation time (T_2) obtained by fitting the sequence of pulses Carr-Purcell-Meiboom-Gill (CPMG) decays to mono-exponential function and multivariate models performed with partial least squares (PLS) were evaluated. The predictability of the PLS model was tested with 10 external samples from another lot. The high linear coefficients (>0.9) and low root means square errors (RMSE) for cross validation and validation proved the applicability of the PLS model.The finding about this study is the TD-NMR CPMG relaxation decays successfully predict total fat on sealed packing of commercial mayonnaises varying in fat content up 10.0 to 55.8 g 100 g^{-1}. The PLS models combined to these signals shown the best results. The main advantage verified is the no-invasive measurement of fat content performed for intact packing of food products. The high linear correlation coefficients between the reference values from Bligh and Byer lipids extraction and those predicted by PLS model evidences the accuracy of multivariate model against the univariate fitting with the discrete T_2 values.

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MO265: Applying NMR relaxometry procedures to characterize and classify soil samples

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The characterization of unsaturated hydraulic properties of soils by using Richard's chamber and van Genuchten phenomenology of water retention are very time consuming methods[1]. By this procedure, many researcher groups treat to describe the dynamics of water molecules in the soils samples. In this description, they take advantage about the dependence of moisture content on different soil water potential, which in some kinds of soils samples takes approximately of some days to many weeks[2].

An alternative and faster procedure is to apply NMR relaxometry protocols and principal component analysis (PCA) technique to perform the classification and characterization in different kinds of soils. The main purpose of this new procedure is to diminish the time of extracting information about characterization and classification of soils samples. To put in practice this idea, we used three different soils with different concentrations of clay, sand and silt[3]. This choice allows us to test the sensibility of this procedure. We compare our results with other well established technique which is the inverse Laplace transform[4].

References:

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[3] F. de C. Balieiro et al., Arvore, Viçosa-MG, 32, 153-162, (2008).

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TU266: Physical and chemical characterization of products petroleum.

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In this work was investigated the application of low field NMR (LF-NMR) to predict physical and chemical properties of petroleum products.

For the tests two Brazilian crude oil were distillated: the crude oil 1 presented TAN = 1.15 mg KOH/g, density of 0.9749 g cm^{-3} and kinematic viscosity 5800 mm2 s^{-1} at 40 °C, and the crude oil 2 with TAN = 1.42 mg KOH/g, density of 0.9164 g cm^{-3} and kinematic viscosity 58.115 mm^2 s^{-1} at 40 °C.

The NMR experiments were performed using a Maran 2 Ultra NMR spectrometer at 2.2 MHz for ^{1}H. The T_2 values was measured using the Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence at 27.5 0C. The CPMG pulse sequence was applied employing $\pi/2$ and π pulses with durations of 8.15 μs and 16 μs, respectively. In the CPMG experiments were recorded 32 transient with 8192 echoes in each transient, one point per echo, echo spacing of 0.2 ms and recycle time of 3s.

The physical and chemical properties as refractive index, kinematic viscosity, total acid number, boiling point, specific gravity were determined directly by standard methodologies ASTM D-1218, D 445-06, D-664-04, D-2892 and D 4052, respectively. The results showed good correlation with the mean values of the transversal relaxation time (T_2).

It can be concluded of this work, that the proposed method for distillated analysis, LF-NMR, presented several advantages as non-destructiveness and not require solvents or dilution. This allows the assessment of several properties simultaneously, based on the output of only one NMR experiment, leading to large economy in terms of energy, time and costs. Thus, it is suggested that the LF-NMR technique can be applied for routine analysis as a guide in the quality control of the distilled products.

ACKNOLEDGEMENTS: CNPq, FAPES, PETROBRAS, LABPETRO DQUI/UFES.

TH267: Influence of the incorporation of fibers in biscuit dough. Characterization by time domain NMR and rheology.

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Several epidemiological and experimental studies show that consumption of determined food products can act either as protective or as risk factors on non-transmissible diseases. Recommendations have emerged that aim to reducing the ingestion of sugars and fats, or to increase the fiber content (particularly soluble) in the diet. Biscuit or cookie dough is a complex system containing abundant components in different states, such as starch, gluten, lipids (flour constituents), sugars, fats and water. In biscuits, both, the incorporation of fibers or the reduction of sugar and fat, create a number of technological problems in processing and in some cases a loss of acceptability [1]. For this reason, the effects on the physico-chemical, rheological and structural characteristics of biscuit dough upon incorporation or reduction of determined ingredients is of great interest in food industry. It is generally known that the distribution of water can affect the rheology of the dough machinability [2]. Low resolution NMR is an important tool as it allows the study of water mobility by means of relaxation time measurements (T_2) in the sample, in a non-invasively, fast and accessible way. In this work we study the proton water mobility in standard biscuit dough through relaxation profiles obtained from a CPMG sequence at 0.5 Tesla. Different populations are assigned to different ingredients [3]. The dependence of mobility as a function

from 40 cm height). The samples were analyzed before and just after the impact, every hour up to 8h, and after 48 hours. All mechanical injuries caused almost instantaneous increases in T_2 values, reaching a peak at about 5h, and then slowly returning to initial value in 48 hours. The increase of T_2 value after the injury is related to reduction of internal oxygen in the fruits, and is direct related to the CO_2 production. When the injured apples were maintained in nitrogen atmosphere, the T_2 values increased more than three times when compared to storage in air. The ratio between the T_2 area of vacuolar and cytoplasmatic water decreased with the severity of injury and it was able to distingue between apples with moderate and severe injuries from non-injured ones. Therefore, TD–NMR protocols has the potential to classify apples according to mechanical injuries incidence and severity.

TU272: Use of TD-NMR to Measure Water Embebition by Seeds Directly in the Soil

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NMR and MRI have been used to measure water content and water transport in soils as well as the water content and distribution in plant roots. Most of these studies are performed in synthetic soil (mixture of sand/silt) or real soils with very low content of magnetic particles. The NMR studies are not well succeeded when the soil has high content of magnetic particles due to the distortion in B0 and the presence of large amount of paramagnetic ions that reduces the relaxation time to the same order of receiver dead time. Here we are showing that the time domain NMR (TD-NMR) can be used to measure the water uptake by seed in moist soil with very high content of magnetic particles. This process is very important because the seed germination begins with water uptake and triggers a series of metabolic changes that culminate in the emergence of the primary root. The CPMG pulse sequence were carried out in a SLK-100 Spinlock spectrometer (model SL.IM.01. The spectrometer uses a 0.23T permanent magnet. It was used soybean (*Glycine max*) and garbanzo bean (*Cicerarietinum*) seeds. The soil used was a typical Brazilian soil and it was moistened to field capacity. In this soil, the water signal was not observed by NMR. Therefore, when seeds were placed in this soil the NMR signals was proportional to the water absorbed by the seed (imbibition process). The seeds in the soil absorb water in lower rate than the seeds in pure water, indicating the influence of the soil ionic force in this process. Therefore TD-NMR can be used to follow the imbibition process in intact seed direct in soil which is not possible with current technologies.

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TH273: Use of Unilateral NMR sensor to Measure Temperature in Intact Seeds and Seeds Inside Soils

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Time domain Nuclear Magnetic Resonance (NMR) has been used as non-contact, non-destructive, no reagent chemical analytical method. In this paper we are showing that we can use time domain Unilateral NMR (UNMR) sensor to measure the temperature of intact oilseeds and oilseed in the soil. The measurement is based on the T_2 dependence of either oil viscosity or temperature. As oil viscosity decreases exponentially with temperature the T_2 value is used to measure temperature in intact oilseeds using a UNMR sensor. Some seeds may survive in high temperature environment for days, but the seedling may die in few hours. Therefore, the seed temperature is an important parameter to agriculture research. The T_2 measurements were carried out in a homemade UNMR. The spectrometer uses a 0.6T (24MHz) home made UNMR sensor and a Tecmag console.

MO274: Estimation of available Water in Soils by NMR Relaxometry

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In soil science it is essential to understand water/soil physicochemical interactions. Traditional procedures to understand these interactions are the measurement of water retention curves and the construction of pedotransfer functions. Both methods give accurate information about soil moisture, but they can be very time consuming depending on the components of soil to be analyzed, including clay, silt and organic matter. Also, normally these measurements offer only bulk data. Soil moisture curves can also be measured by NMR relaxometry, following wetting and dewetting procedures. In this case, the curves can be obtained in a faster way and the physicochemical interactions between water and the various soil components normally result in different average T_2 values, allowing obtaining water retention curves for each specific soil component, being more informative when compared with bulk measurements. In order to measure water retention curves by NMR, we used three different soils: top soil layer of Abruptic Arenic Ochraquult, as well as top and deeper layers of Abruptic Aquic Arenic Hapludult, that differ in terms of composition and particle size distribution. The samples were drained in a controlled way using the moisture pressure plate extractor (Richards chamber), which dries the soil by increasing the internal chamber pressure. NMR experiments were performed at room temperature using a TECMAG LapNMR console, a 620-Gauss permanent magnet, and a homemade NMR probe. T_2 relaxation times were obtained from CPMG experiments as a function of drained water for all the samples, using draining pressures of 1, 3, 5, 9, 13, 20, 40, 60, and 80 psi. From the T_2 curves obtained versus draining pressures for each soil, different water retention behaviors were observed. These results reflect the different interactions of water with the various soil components, showing the applicability of this method to differentiate soils by their specific water retention capability and composition. This work indicates how NMR relaxometry can be used as an alternative method to obtain water retention curves.

AKNOWLEDGEMENTS: IFSC/USP, FAPESP, CNPq, and CAPES.

TU275: Compact, Cryogen-Free, High-Resolution 60 MHz Permanent Magnet NMR Systems for Reaction Monitoring and On-Line/At-Line Process Control Observing ^{1}H, 19F, ^{31}P

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A compact high resolution NMR system will be described that can be situated on the bench-top or in the fume hood to be used as a continuous or stop-flow detector and/or an "in-situ" reaction monitoring system. The same system can be fully integrated into on-line shelters for on-line process control or utilized by engineers and technicians in an "at-line" environment. The system uses a unique 1.5 Tesla permanent magnet that can accommodate sample tube diameters of 3-10 mm with half-height spectral resolution (water resonance) approaching 1-3 Hz depending on the sample volume size and with excellent single pulse sensitivity. These systems can be utilized in a traditional NMR methodology approach or combined with chemometric approaches that allow NMR