Determination of fat and moisture contents by time-domain NMR

A first-year student project, presumably for the summer of 2022

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The term 'time-domain NMR' (TD-NMR) refers to the NMR methods that do not aim at obtaining Fourier-transformed frequency spectra but provide information from the dependence of signal intensity on time, *i.e.*, from the 'raw' data. The TD-NMR arsenal includes echo-based experiments, spin-diffusion experiments and gradient experiments. The echo-based experiments, in particular, allow one to discriminate between sample's constituents with different molecular mobility, as reflected in their T_1 and T_2 relaxation rates. The workhorse of this method is a Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence which provides a multi-echo signal in a single shot. To quantify the signal's components decaying with different T_2's, a multivariate regression analysis is applied. In particular, a classical least squares (CLS) calibration is a method of choice when the characteristic T_2's of the sample's constituents are invariant within the given sample set (Fig. 1).

Another way to quantify distinct-T_2 constituents is Inverse Laplace Transformation (ILT) of the decay. The ILT is a mathematical algorithm that searches for a multi-exponential function of best fit to the data, the result being presented as a histogram showing a T_2 *distribution* in the sample. In the best scenario, the distribution is resolved into separate peaks that are easy to integrate. If it does not provide sufficient resolution, different relaxation components can be revealed and quantified through a two-dimensional (2D) ILT applied to a series of T_1-weighted CPMG signals (Fig. 2).

An interested student will learn these methods running CPMG experiments on food samples, using a high-field NMR spectrometer (Bruker Avance III). To learn the CLS calibration analysis, several calibration samples with a known concentration of the component of interest will be prepared. The samples may be either synthetic ones (*e.g.* oil-in-water emulsion in agar gel), or of natural origin (*e.g.* cheese or other dairy product with different fat content).

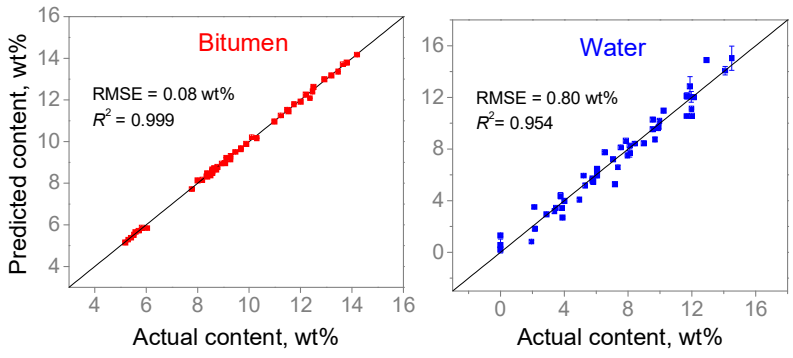

Fig. 1. Quantitation of bitumen and water in 50 bituminous sands through a CLS calibration analysis of CPMG decays.

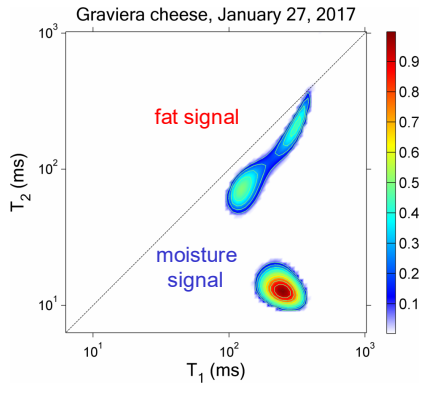

Fig.2. 2D ILT showing a T_1-T_2 distribution in a young Graviera cheese. Water and fat components are well resolved and can be quantified directly from the ILT intensities.