Parameterization of multi-exponential NMR relaxation in terms of logarithmic moments of an underlying relaxation time distribution

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There are two common approaches to the mathematical description of multi-exponential relaxation. One is to fit an empirical function whose parameters relate to a characteristic time of relaxation and its deviation from exponential. Kohlrausch-William-Watson, Cole-Cole, Cole-Davidson and log-normal fit functions are but some of the examples. This approach requires specifying a functional form of relaxation, or in other words, *a priori* knowledge of underlying relaxation time distribution $g(\tau)$, which makes it difficult to compare samples with dissimilar relaxation behavior using this method. The other approach is calculation of $g(\tau)$ by resolving an experimental relaxation function into a number of exponentials by means of the inverse Laplace transform (ILT). It provides an ultimate description of the multi-exponential relaxation and allows a direct comparison of different samples. However, since ILT of a noisy data is a numerical approximation and relies strongly on the regularization algorithm used, one may consider thus obtained $g(\tau)$ and derived moments ambiguous.

R. Zorn [1] has proposed to characterize multi-exponential relaxation in terms of logarithmic moments (LMs) of $g(\tau)$ which can be calculated without inversion of data by using only integral (and optionally differential) calculus. The first logarithmic moment, $<\ln\tau>$, represents the geometric mean relaxation time, wihle the second, $\sigma^2_{\ln\tau}$, and the third, $\mu_{3\,\ln\tau}$, moments relate to the width and the asymmetry of $g(\tau)$, respectively. The calculation of the LMs is based on the moment rules for convolution (see *e.g.* [2]) and requires that a relaxation function is sampled at logarithmically spaced delays and normalized to unity.

Ref. [1] contains all necessary equations for the LMs calculation and provides examples for a number of empirical fit functions used in dielectric relaxometry. Here we have applied the method to experimental data acquired under various conditions from NMR T_1 relaxation and stimulated echo experiments as well as to simulated data. In particular, we tested the effects of a signal-to-noise ratio (SNR), the number of acquisition points, the onset of acquisition, and a sampling rate on the calculated LMs. It was possible to exclude a numerical differentiation from the working equations in [1], which left numerical integration and normalization of the data the only intrinsic sources of error. To normalize the data, we used the total amplitude of the best-fit triple-exponential function as a normalization factor. The same fit function was utilized to extrapolate the relaxation function to short relaxation delays if necessary.

The LMs calculated from the experimental datasets were found in a good agreement with those from ILT (UPEN) and multi-exponential analysis. The geometric mean $<\ln\tau>$ is robust with respect to the presence of noise, including outliers, to a moderate shift of the acquisition onset to longer delays, and to its early truncation. The variance $\sigma^2_{\ln\tau}$ and the asymmety parameter $\mu_{3\,\ln\tau}$ were found to be much more sensitive to those factors. For example, it was important for a good accuracy that the relaxation decay be sampled starting above a 90% level of the relaxation function, otherwise extrapolation to short delays was necessary.

This work is one of objectives of EU programme "Improving diagnosis by fast field-cycling MRI" (IDentIFY). It is intended for developing a reliable algorithm for parameterization of non-exponential relaxation processes, in order to establish a common basis for characterizing relaxation in bio-tissues and possibly to increase the contrast in T_1 dispersion measurements.

References

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