T_1 Relaxation Time Distribution Inversion: Reinvented

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Introduction: Multi-exponential recovery is prevalent in T_1 relaxation processes in NMR and MRI where a signal recovers through multiple relaxation processes to an equilibrium steady-state value. In heterogeneous materials, these processes exhibit a complex behavior reflecting the eigenvalues of relaxation-diffusion and exchange processes that is better represented by a probability distribution function $f(\tau)$ of lifetimes, as

$$s(t) = \int_0^\infty f(\tau)\,\left(1 - \alpha\, e^{-\frac{t}{\tau}}\right) d\tau. \qquad \text{Eq. 1}$$

The goal of T_1 relaxation time distribution inversion is to compute $f(\tau)$ from signal $s(t)$.

Methods: Eq. 1 is commonly solved for $f(\tau)$ by two schemes by either (a) fitting the data to a pre-defined mathematical model with assuming a fixed value of $\alpha = 2$ or $\alpha = 1$ [1], or (b) normalizing the signal in the positive real space and employing methods designed for multi-exponential decay [2]. We recognized that these schemes are not appropriate or efficient – especially in inhomogeneous radiofrequency fields, for quadrupolar nuclei, and for samples with long T_1. We provide a robust alternative solution to finding $f(\tau)$ in multi-exponential *recovery* processes with *unknown recovery factor* α and *without extended measurement windows*. By recasting the recovery signal as a linear system,

$$s(t) = \sum_{i=0}^{N_\tau}[f_i - \alpha f_i \exp(-t/\tau_i)] = f_\infty - \sum_{i=1}^{N_\tau} f_i' \exp(-t/\tau_i), \qquad \text{Eq. 2}$$

that includes the unknown steady-state value f_∞ explicitly, and the recovery factor α implicitly, we solve for f_i' and f_∞ by employing regularization – and finally obtain the lifetime distribution f_i corresponding to τ_i.

Results and discussion: The invented method performs an excellent inversion even for non-ideal recovery factors and short measurement windows; see Fig. 1. We applied the method, and will show its results, in NMR spectroscopy of milk powders and crude oil, surface NMR of aquifers, and dynamic nuclear polarization – where it showed interesting results that would not be obtained without.

The method can detect lifetime components approximately at the same order of magnitude as the longest measurement time. The recovery factor appropriately captures instrument and sample non-idealities and folds these imperfections into a fitting parameter with physical significance.

Conclusion: The revised formulation finds $f(\tau)$ in any one- or multi-dimensional datasets with at least one recovery dimension in NMR, MRI, surface NMR, and dynamic nuclear polarization build-up curves – completely transforming how we process T_1 recovery data and distinguishing it from multi-exponential decay analysis.

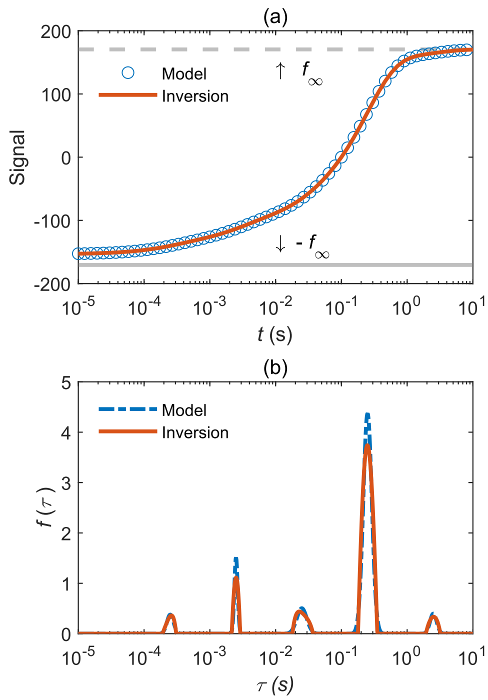

Fig. 1: Excellent agreement was found between the model and its inversion for non-ideal cases; here with recovery factor $\alpha = 1.9$ and a signal that is still rising at the longest measurement times.

References: [1] Venkataramanan, IEEE Trans. Signal Process. (2002). [2] Afrough, Phys. Rev. Applied (2021).