# 3TM software for NMRD data fitting with the 3-Tau Model [1]

*Data-Sheet*

The 3TM [1] is a standalone software based on the 3-Tau model [**2,3,4**], suitable for fitting the NMRD profiles of a wide variety of porous media. It has been developed in the Matlab App Designer™ environment.
The 3TM sw is user-friendly and equipped with a practical interface that allows the user to plot and fit the NMR dispersion profiles obtained from Fast Field Cycling experiments.

Main features:

1) The **3TM sw** can be successfully used to fit NMR dispersion data obtained from many different kinds of samples with average pore sizes ranging from around 10 nanometers to micrometers, and with different kinds of fluids:
   - water
   - petroleum and its derivatives
   - alcohols

2) The **3TM sw** provides best-fit solutions (using a least-squares minimization algorithm) in terms of 3 physical parameters ($\tau_l$, $\tau_d$, $\tau_b$) that can be used to characterize the sample being studied:
   - $\tau_l$ – diffusion correlation time for spins within the layer
   - $\tau_b$ – diffusion correlation time for spins in the bulk
   - $\tau_d$ – desorption correlation time for spins from the surface layer to the bulk

   The ratio $\tau_d / \tau_l$ represents the number of hops that a molecule of water makes at the surface of the pore before desorption. This number can provide supplementary information about the *surface affinity* of the fluid.

3) The **3TM sw** allows the user to choose between 3 different kinds of interactions:
   - HH – homonuclear interaction (proton-proton)
   - HM – heteronuclear interaction (proton-paramagnetic centres)
   - HH+MH – both the homonuclear and the heteronuclear interactions

4) Fields of application of the **3TM sw:**
   - hydrated cementitious materials
   - clays and rocks (applications as safe repositories for radioactive wastes)
   - catalysts
   - silicates (for example in pastes)
   - hydrocarbon-bearing rock
   - food products (such as cheese)
   - wood and plants
   - soil / environmental studies
   - particle suspensions, pastes, creams and slurries

## REFERENCES:

[**1**] Kogon, R., & Faux, D. (2022). 3TM: Software for the 3-Tau Model. *SoftwareX*, *17*, 100979.
[**2**] Faux, D. A., & McDonald, P. J. (2017). Explicit calculation of nuclear-magnetic-resonance relaxation rates in small pores to elucidate molecular-scale fluid dynamics. *Physical Review E*, *95*(3), 033117.
[**3**] Faux, D. A., McDonald, P. J., & Howlett, N. C. (2017). Nuclear-magnetic-resonance relaxation due to the translational diffusion of fluid confined to quasi-two-dimensional pores. *Physical Review E*, *95*(3), 033116.
[**4**] Faux, D., Kogon, R., Bortolotti, V., & McDonald, P. (2019). Advances in the interpretation of frequency-dependent Nuclear Magnetic Resonance measurements from porous material. *Molecules*, *24*(20), 3688.