European Union's HORIZON-MSCA-2022-SE-01-01 – MSCA Staff Exchanges
2022 program, Grant agreement 101131564 (project "NMR_IMPROV")

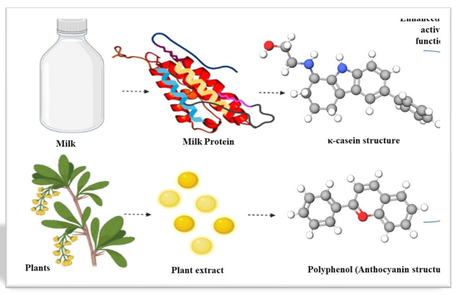
NMR Relaxation as a Tool for Investigating the Molecular Behavior of Plant-Derived Food Matrices

Faisal Sheraz Shah[1], Kacper Gorski[2], Pedro J. Sebastião[3], Özlem Özmutlu Karslioglu[4], Danuta Kruk[1*]

[1]*Department of Physics and Biophysics, University of Warmia and Mazury in Olsztyn, Oczapowskiego 4, 10-719 Olsztyn, Poland*
[2]*Department of Chemistry, University of Warmia and Mazury in Olsztyn, Plac Łódzki 4, Olsztyn 10-727, Poland*
[3]*CeFEMA and Department of Physics,Instituto Superior Técnico, University of Lisbon, 1049-001Lisbon, Portugal*
[4]*Institute of Food Technology, University of Applied Sciences Weihenstephan-Triesdorf, Am Staudengarten 11, 85354 Freising, Germany*

Introduction

- Plant-based dairy alternatives, such as plant-based milk and yogurt, have gained popularity due to their nutritional, environmental, and ethical advantages.
- However, these systems are physically and chemically complex, often involving emulsions, polysaccharides, proteins, and various bioactive compounds that affect their stability, texture, and sensory attributes.
- To ensure product quality and shelf-life, it is essential to understand the molecular dynamics and water mobility within these matrices.
- Fast Field Cycling Nuclear Magnetic Resonance (FFC NMR) relaxometry provides insights into molecular motion across a wide range of time scales by analyzing longitudinal relaxation rates $R_1=\frac{1}{T1}$as a function of magnetic field strength (NMRD profiles). This makes FFC NMR especially valuable in studying hydration, mobility, and matrix interactions in semi-solid and gel-like systems such as plant-based yogurts.



Objective

The objective of this study is to apply Fast Field Cycling (FFC) NMR relaxometry to investigate the molecular mobility and water–macromolecule interactions in plant-based milk and yogurt. The aim is to characterize how plant proteins, polysaccharides, and emulsifiers influence the internal dynamics and structural organization of these matrices. This approach will help link molecular level behavior to key functional properties such as texture, water binding capacity, and product stability, ultimately supporting the development of improved plant-based dairy alternatives.

Theory and Experimental Results

We used two diffusion contributions with one *BPP* for rotations as a theoretical model to made the fits and get the required parameters and is given as:

$$R_1^{Total}(\omega_L) = R^{BPP}(\omega_L,\tau_R) + R_1^{SD}(\omega_L,\tau_{D1}) + R_1^{SD}(\omega_L,\tau_{D2}) \quad (1)$$

$$R_1^i(\omega,\tau) = A^i[\,J^i(\omega,\tau) + 4\,J^i(2\omega,\tau)] \quad (2)$$

$$i \equiv BPP;\ SD$$

$$J^{BPP}(\omega,\tau) = \frac{\tau}{1+\omega^2\tau^2} \quad (3)$$

This relaxation rate was first obtained by N. Bloembergen, E. M. Purcell, and R. V. Pound and is often denoted the *BPP* relaxation model (Eq.3).

The spectral density for the self diffusion contribution of the Freed model is expressed in Eq.4.

$$J^{SD}(\omega,\tau) = 72\,\frac{3}{4\pi}\int_0^\infty \frac{\mu^2}{81-9\mu^2-2\mu^4+\mu^6}\,\frac{\mu^2\tau}{\mu^4+(\omega\tau)^2}\,d\mu \quad (4)$$

$$\tau_D = \frac{d^2}{2D}$$

τ is the correlation time, ω is the Larmor angular frequency, A denotes an effective dipole-dipole coupling constant. The parameter d is the distance of closest approach of the interacting nuclei.

Tab.1. Parameters obtained by fitting the relaxation dispersion data in terms of Equation (1).

Label	T[K]	chi²t	NP	n	reff [m]	τ_1[s]	d [m]	d_1 [m]	D [m²/s]	D_1 [m²/s]
Alpro_Milk	298	1.7676	10	6.68×10^{28}	3.10×10^{-10}	5×10^{-10}	5.66×10^{-10}	3.57×10^{-9}	3.88×10^{-11}	2.34×10^{-12}
Yogurt_Alpro	298	1.6615	10	4.00×10^{28}	2.70×10^{-10}	9.91×10^{-10}	3.51×10^{-9}	1.34×10^{-9}	1.17×10^{-12}	8.84×10^{-12}
Vemondo_Coconut	298	2.4407	10	6.68×10^{28}	3.10×10^{-10}	5×10^{-10}	9.00×10^{-9}	2.26×10^{-9}	2.88×10^{-11}	1.01×10^{-10}
Vemondo_Yogurt	298	1.245	10	4.00×10^{28}	3.10×10^{-10}	7.59×10^{-10}	5.64×10^{-9}	2.07×10^{-9}	3.39×10^{-12}	2.02×10^{-11}

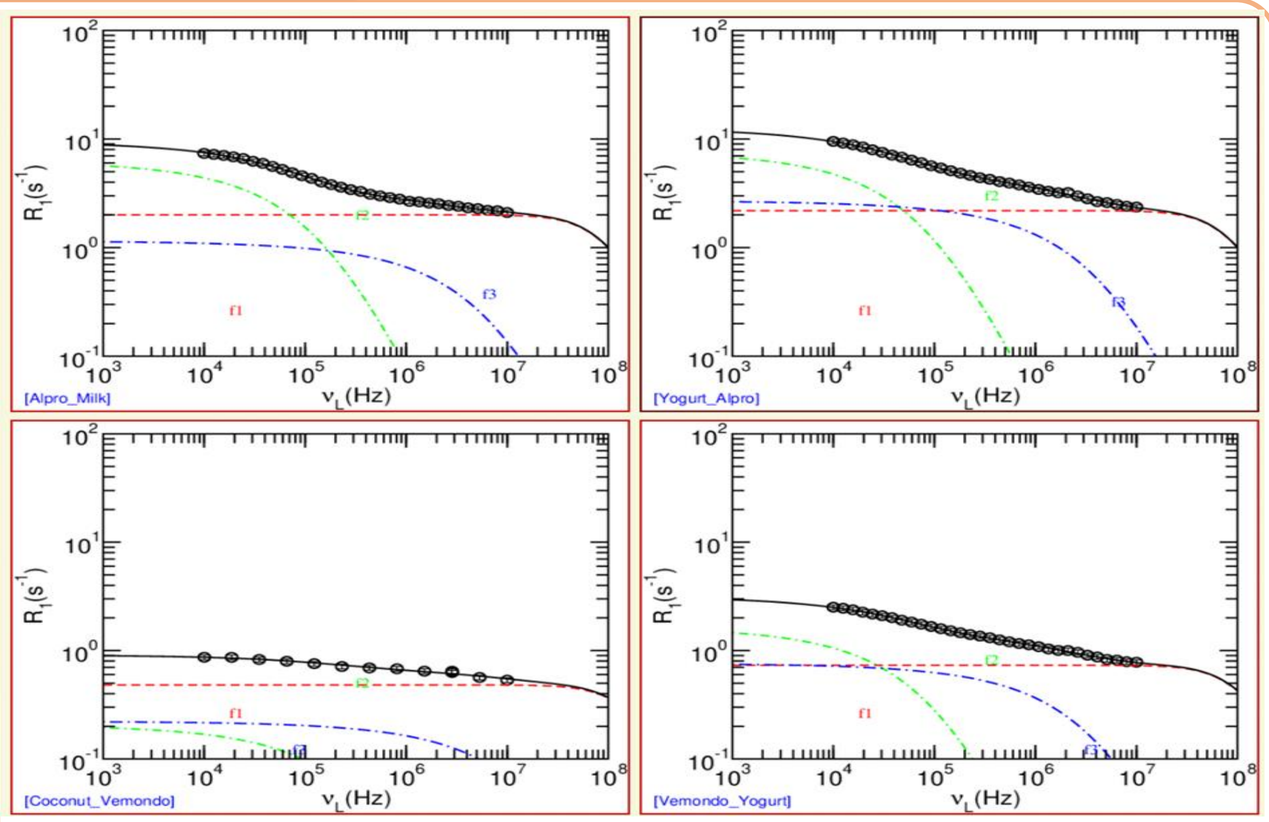


Fig.1. Relaxation dispersion data of commercially available Soya based Alpro Milk and yogurt, and coconut based Vemondo milk and yogurt at T = 298 K for all. Fits of the overall relaxation rate in terms of Equation (1). The parameters are given in Table 1.

Conclusions

The relaxation behavior of plant-based milk and yogurt was explained using a model that combines using a model that includes a BPP-type contribution along with two distinct diffusion-related terms associated with the particle's mobility. This model worked well across different magnetic field strengths, especially when the size of the particles in the sample was similar. For samples with a wider range of particle sizes, the results could still be understood by assuming the presence of two main types of particles with different sizes and movements. This approach helped reveal how the internal structure and composition of plant-based products affect their molecular dynamics.

References:

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