HOW TO GET WATER DIFFUSION COEFFICIENT FOR HYRATED PECTIN - INSIGHT FROM NMR RELAXOMETRY

***Hatice Gul Solmaz*[a], Maciej Osuch[b], Aylin Ozgur[a], Mecit Oztop[c], Danuta Kruk[b]**

[a]Kayseri Seker A. S., Seker Mahallesi Osman Kavuncu Bulvari NO: 314, Kocasinan/KAYSERI, Turkey,
hatice.solmaz@kayseriseker.com.tr, aylin.ozgur@kayseriseker.com.tr
[b]Faculty of Mathematics and Computer Science, University of Warmia and Mazury in Olsztyn, Sloneczna 54, 10-710 Olsztyn, Poland, maciej.osuch@uwm.edu.pl, danuta.kruk@uwm.edu.pl
[c]Department of Food Engineering, Middle East Technical University, Ankara 06800, Turkey,
mecit@metu.edu.tr

1. Introduction

Pectin is used in food industry as gelling agent, thickener, and stabilizer in jams, jelly, fruit juices, bakery, milk and confectionary product. Commercial pectin sample are extracted from citrus peel and apple pomace in most instances, and pectin is also obtained from sugar beet pulp.

Aim : obtaining water diffusion coefficient for hydrated pectin with NMR Relaxometry and to define the amount of water confined within gel structure.

2. Material and Methods

The pectin sample used in the study containss 30% maltodextrin and was produced in the Kayseri Seker Factory, Kayseri, TURKEY. Two different sample concentrations were used, **10 %** and **20 %.**

^{1}H spin-lattice relaxation experiments have been performed in the frequency range from 10 kHz to 100 MHz at **25 °C , 35 °C** and **45 °C**.

3. Results

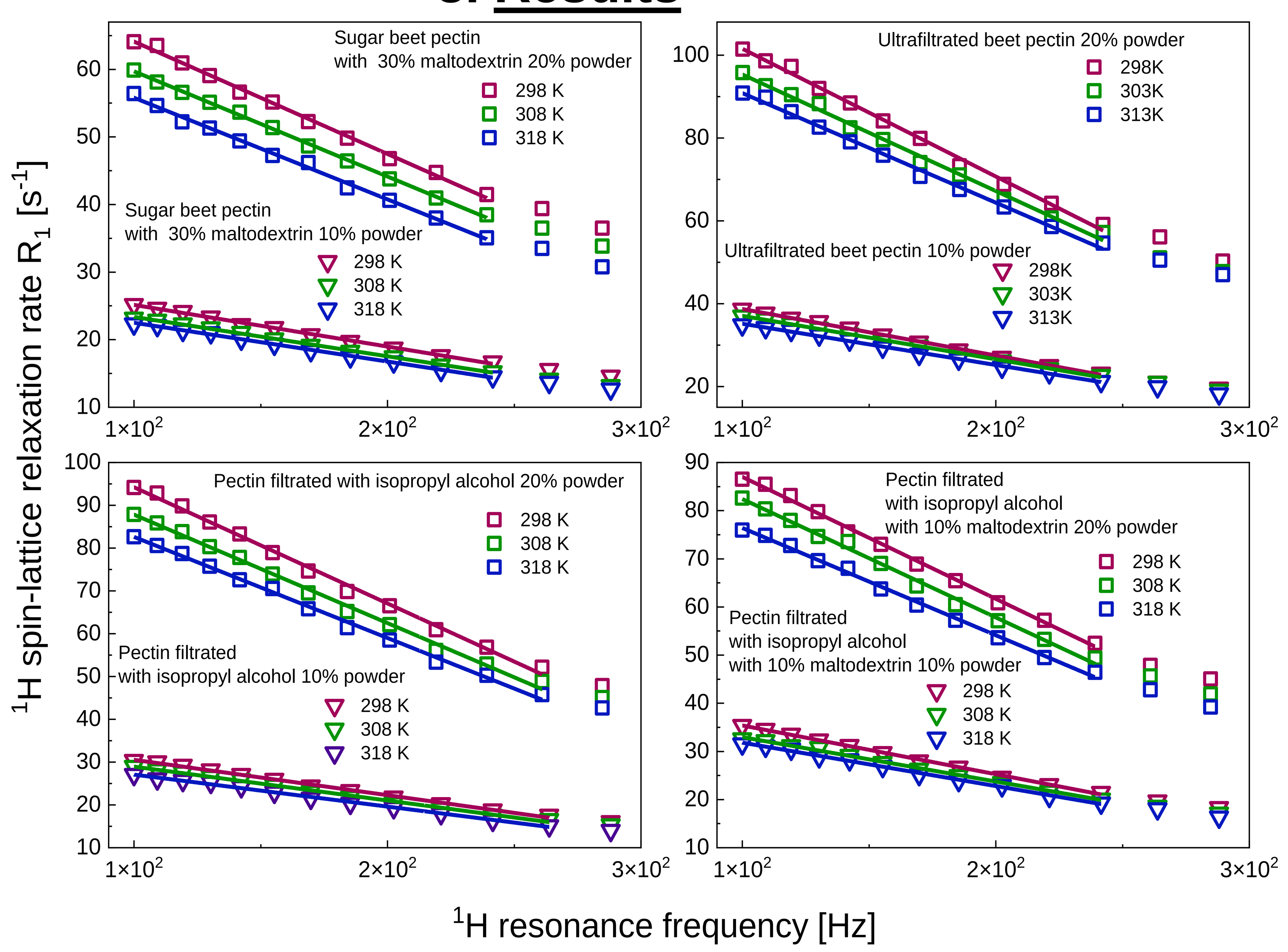

Fig 1. ^{1}H NMR relaxometry data for hydrated pectin versus square root of the resonance frequency.

5.Model of Water Dynamics

Magnetic dipole-dipole interactions that can be of intramolecular or intermolecular origin cause ^{1}H relaxation processes. The intramolecular and intermolecular relaxation contributions, denoted as R_1^{intra} and R_1^{inter} constitute the overall relaxation rate R_1.

$$R_1(\omega_H) = R_1^{intra}(\omega_H) + R_1^{inter}(\omega_H)$$

$$R_1^{inter}(\omega_H) = \frac{108}{5}\left(\frac{\mu_0}{4\pi}\gamma_{H^h}^2\right)^2 \frac{N_H}{d^3}\int_0^\infty \frac{u^4}{81+9u^2-2u^4+u^6}\left[\frac{\tau_{trans}}{u^4+(\omega\tau_{trans})^2}+\frac{4\tau_{trans}}{u^4+(2\omega\tau_{trans})^2}\right]du$$

$$R_1^{intra}(\omega_H) = C^{DD}\left[\frac{\tau_{rot}}{1+(\omega\tau_{rot})^2}+\frac{4\tau_{rot}}{1+(2\omega\tau_{rot})^2}\right]$$

C^{DD}- dipolar relaxation constant

τ_{rot} - rotational correlation time

$\tau_{trans} = \frac{d_{cc}^2}{D_{trans}^{cc}}$

d_{cc} - cation-cation distance of closest

D_{trans}^{cc} - relative, cation-cation translation diffusion coefficient

N_H - numbers of ^{1}H nuclei per unit volume

ω_H - resonance frequency

6. Conclusions

Translational diffusion coeffcients of water confined in pectin matrices ranges from $1.92*10^{-13}$ at 298K to $2.03*10^{-13}$ at 318K.

The number of water protons per unit volume obtained from the analysis is of the order of $5.54*10^{27}$ This implies that the fraction of confined water molecules is of the order of $x=5.54*10^{27}/6.7*10^{28}=0.092$ ($6.7*10^{28}$ – number of hydrogen atoms per m^3 in bulk water)

4. Analysis

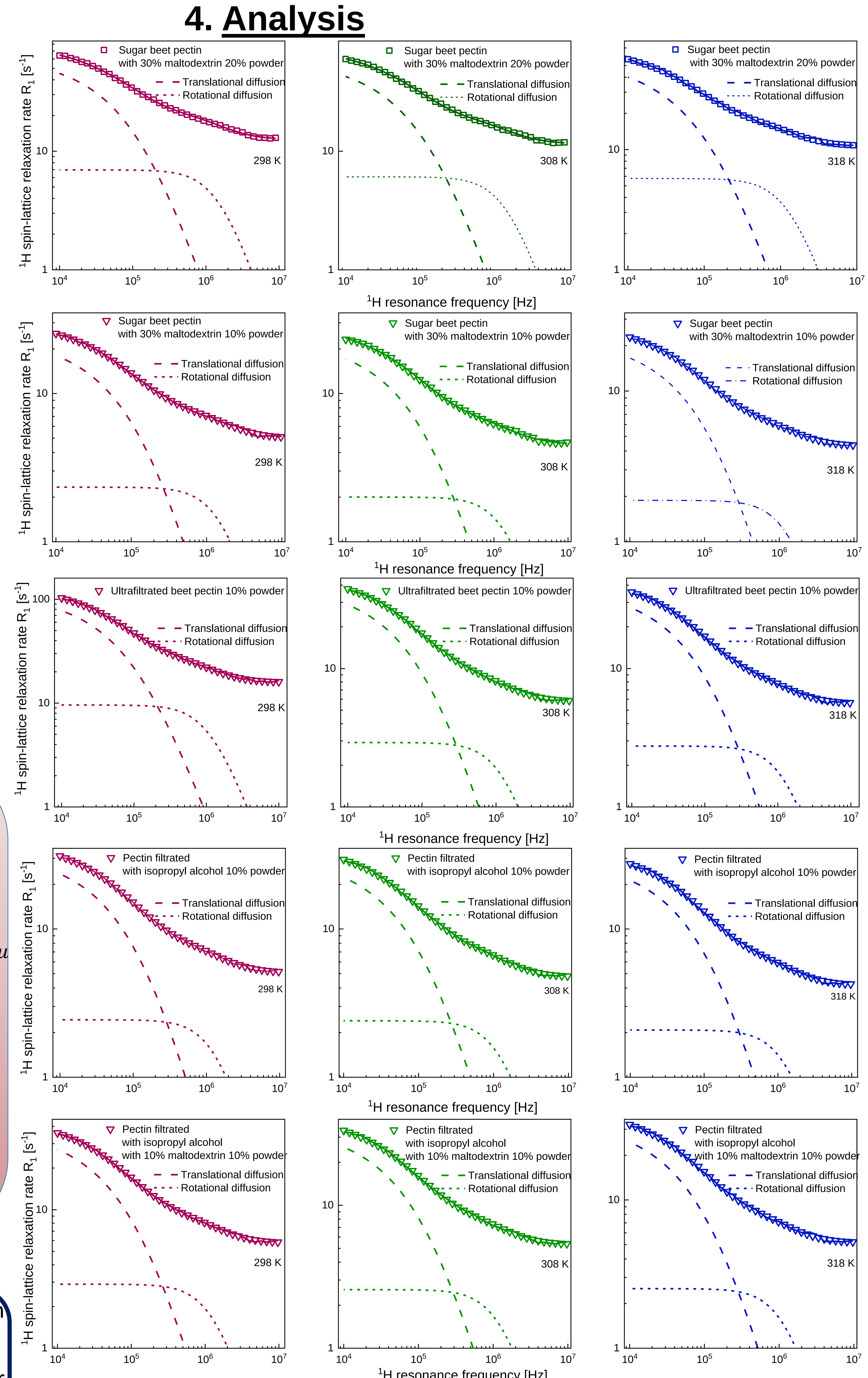

Fig 2. Decomposition of ^{1}H spin lattice relaxation data into relaxation contributions associated with translational and rotational diffusion of water- dashed and dotted lines, respectively.

6.References

[1] D. Kruk, M. Wojciechowski, Y.L. Verma, S. K. Chaurasia, R.K Singh, Phys. Chem. Chem. Phys. 19, 32605 (2017).
[2] D. Kruk, E. Masiewicz, S. Lotarska, R. Markiewicz, S. Jurga, Int. J. Mol. Sci. 23, 1688 (2022).
[3] R. Meier, D. Kruk, A. Bourdick, E. Schneider, E.A. Rössler, Appl. Magn. Reson. 44, 153 (2012).
[4] R. Meier, D. Kruk, J. Gmeiner, E.A. Rössler, J. Chem. Phys. 136, 034508 (2012).
[5] D. Kruk, R. Meier, E.A. Rössler, J. Phys. Chem. B 115, 951 (2011). l
[6]Kaya, B., 2020. Extraction Of Pectin From Sugar Beet Pulp By High Hydrostatic Pressure And İnvestigation Of Extraction Efficiency And Extract Characteristics. The Graduate School Of Natural And Applied Sciences Of Middle East TechnicaUniversity, The Degree Of Master Of Science In Food Engineering, p.196

7. Acknowledgements

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 101008228 (project SuChAQuality).

SuChAQuality

Funded By the European Union