

Accelerated porous structure determination of biocompatible hydrogels by Time-Resolved Restricted Diffusion NMR method

M. Czarnota^a, S. Domański^b, M. Urbańczyk^a

^aInstitute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland,

^bPolbionica S.A., Warsaw, Poland

Introduction: Restricted diffusion measurements with Nuclear Magnetic Resonance spectroscopy provide useful information about porous structures. A disadvantage of this measurement is its duration, which can be shortened significantly by applying fast methods [1]. Restricted diffusion measurements utilize the behavior of molecules with movement limited by porous structures since the diffusion coefficient is lower than expected for unrestricted movement. An example of a porous structure can be a gelatin methacrylate (GelMa) hydrogel. GelMa is a biocompatible material that has plenty of applications in medicine. One of the most promising applications is as a scaffold for bionic organs such as the pancreas [2].

Methods: We use Time-Resolved Diffusion NMR to accelerate Restricted Diffusion measurements of GelMa hydrogel samples with varying GelMa concentration, its degree of substitution with methacrylic groups, and illumination time. We also used Scanning Electron Microscopy to compare the results from both methods.

Results and discussion: We obtained the diffusion coefficient of water dependence on diffusion time for GelMa hydrogel samples. The measurement time for a single sample was between 50 minutes and 3 hours, depending on the T_1 relaxation time of water in the sample. In this case, the measurement time was about 14 times shorter than the conventional one with the same resolution of diffusion time dimension. The estimated average size (diameter) of pores is in the range of 60-95 μm . The size was calculated from surface-to-volume ratio (S/V) from the short time ($<100\text{ms}$) dependence of diffusion coefficient (D) on diffusion time (Δ) [3]:

$$\frac{D(\Delta)}{D_0} = 1 - \frac{4}{9\sqrt{\pi}} \times \frac{S}{V} \times \sqrt{D_0 \Delta} \quad D_0 - \text{unrestricted diffusion coefficient} \quad \text{Eq. 1}$$

Assuming that pores are spherical, which was validated by SEM, the diameter can be calculated from S/V . From the $D(\Delta)$ dependence over the whole range of Δ [3]:

$$\frac{D(\Delta)}{D_0} = 1 - \left(1 - \frac{1}{\alpha}\right) \frac{c\sqrt{\Delta} + \left(1 - \frac{1}{\alpha}\right)\frac{\Delta}{\theta}}{\left(1 - \frac{1}{\alpha}\right) + c\sqrt{\Delta} + \left(1 - \frac{1}{\alpha}\right)\frac{\Delta}{\theta}} \quad \theta - \text{pore scaling constant} \quad \text{Eq. 2}$$

$$c = \frac{4}{9\sqrt{\pi}} \times \frac{S}{V} \times \sqrt{D_0}$$

the tortuosity (α) values were calculated.

Conclusion: We were able to accelerate the Restricted Diffusion measurements successfully. By using the Time-Resolved method, GelMa hydrogel's properties can be acquired much faster, about 14 times.

References: [1] Urbańczyk, Anal. Chem. (2020). [2] Klak, Micromachines (2020). [3] Latour, J. Magn. Reson. (1993)