Dehydration analysis of poly-ethylene glycol hydrogels with terahertz imaging

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Abstract: Polyethylene glycol (PEG) hydrogel are commonly used as both scaffolds and drug delivery systems to aid in cellular differentiation, thus developing a good understanding of their water properties is key to PEG optimisation. Terahertz (THz) imaging has previously been used to analyse the water content inside polymer films in ambient environment. Here, we apply this approach to extract the desorption profiles of PEG hydrogels of four concentrations producing results that indicate confinement effects due to porosity on the diffusional properties of water. These preliminary data therefore highlight the broad applicability of THz imaging for the analysis of water properties of PEG hydrogels.

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1. Introduction

Polyethylene glycol hydrogels are utilised in numerous applications and have been demonstrated to have valuable usage in a range of scientific fields, such as 3D scaffolding networks or use as a drug delivery system for cellular differentiation [1, 2]. Given their hydrophilic nature and in view of applications in which water swollen PEG hydrogels contact surfaces, such as in wound repair, drug delivery on skin and art restoration, there is a need to understand water transport and diffusional properties during absorption and desorption. Terahertz radiation is situated on the electromagnetic spectrum between 100 GHz and 30 THz and can penetrate through dielectric materials, such as polymers, but is strongly absorbed by polar materials, such as liquid water. As such, it has been used to quantify water in polymers by spectroscopic means [3] or using focal plane array terahertz imaging [4, 5]. In this work, we build on our earlier demonstrations and applying it to PEG hydrogels where we show that diffusional properties can significantly deviate from simple Fickian diffusion in the presence of small-scale porosity.

2. Methodology

10 mg of PEG hydrogels prepared from 4 different PEG concentrations in solution, namely 12 (p12), 16 (p16), 20 (p20) and 30 (p30) wt%, with average pore size decreasing for increasing PEG content, were placed in a custom-made water cell, rehydrated and allowed to swell until the point that the equilibrium water content had been reached. Two repeats were taken for each concentration. Desorption profiles of the samples in the ambient environment were then imaged using the THz imaging system [3, 4] while weight measurements were also acquired. The acquired average THz intensity profiles were then converted to mass (mg) for comparisons against weight measurements. The diffusion coefficient was calculated by fitting the measured relative variation of mass due to swelling, m* (t) with a law describing effective diffusion, $m^{*}(t) \approx k_{eff}t^{n}$, with n = 0.5 for Fickian diffusion [6], and n > 0.5 for sub diffusion. An effective diffusion coefficient was extracted as $D_{eff} = {k_{eff}}^{2}l^{2}\pi/16$ with l being the thickness of the sample.

3. Results/Discussion

Figure 1 compares THz data against the weight data where a good agreement can generally be observed. Furthermore, statistical significance for the data set was demonstrated with a statistical probability, P-value of $P \leq 0.05$. As expected, the shape of desorption profile follows the concentration profile consistent with [6] that generally displays a decrease in water content, a reflection of a decrease in pore size, in respects to an increase in PEG concentration. However, one exception is the p20 sample - despite being an intermediary concentration, it had the largest desorption profile. This is possibly due to environmental influences resulting in thickness discrepancies. Fig 2a shows THz data plotted as m* (t) as a function of √t: only the smallest concentration sample p12 shows a linear dependence compatible with Fickian diffusive behaviour (n=0.56). However, the diffusion coefficient is significantly smaller than for bulk water, indicating the effect of porous confinement. All remaining samples show sub-diffusive behaviour (Fig.2b), as indicated by n > 0.5. Up to p20, the value of n increases and

D_{eff} decreases with increasing PEG content (decreasing pore size), consistent with a more pronounced confinement. The data for P30 seem to indicate an inversion of the trend, that needs further investigation.

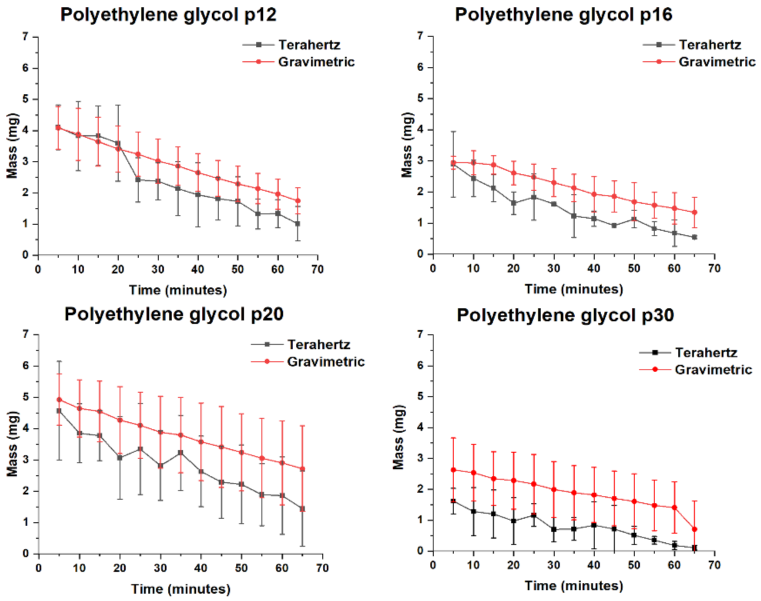

Figure1 The results of the H_2O dehydration of the PEG samples. Plotted on the y axis is the H_2O mass taken at 5-minute timepoints as plotted as a function of time on the x-axis.

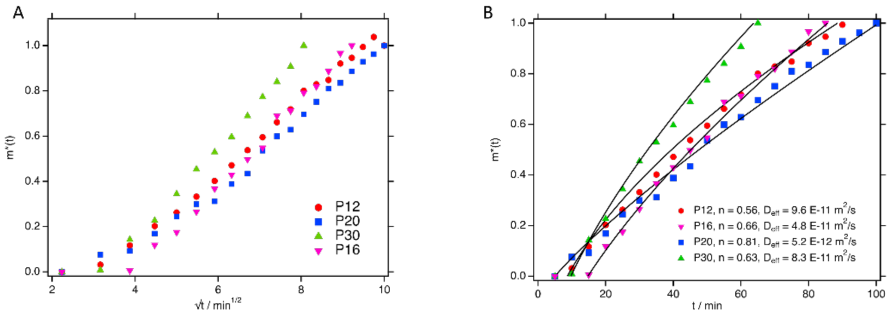

Figure 2 The results of the qualitative analysis a) represents $m^*(t)$ as a function of $\sqrt{t}$ and shows the linearity of p12 in line with Fickian diffusion. Graph b) plots $m^*(t)$ as t/min and illustrates the result of the fitting analysis, with again variant p12 compatible with diffusion.

4. Conclusion

Although in its infancy, demonstrated here was the potential of THz imaging to quantitatively analyse the relative water mass of PEG hydrogels and thus analyse their diffusional properties. The results presented a good correlation between the THz and the gravimetric analysis. Additionally, demonstrating a statistically significant difference between the concentration variables.

5. Acknowledgements

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6. References

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