Diffusion in aqueous solutions of poly (ethylene glycol) : Pulsed Field Gradient NMR measurements

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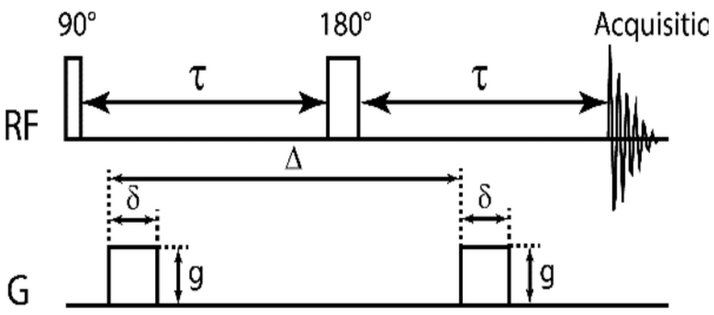
Abstract

Poly (ethylene glycol) (PEG) is a non ionic polymer which has been used as a probe polymer in constructing a model system for macromolecular crowding in cells [1]. Macromolecular crowding in cells is thought to result from the excluded volume effect, although other non-specific effects (such as electrostatics) are likely important as well. In this study, we investigate the dynamics of aqueous solutions of this model polymer using pulsed-field-gradient NMR using gradients much larger than in the previous study. Our preliminary observations suggest a bi-exponential signal decay as a function of the gradient intensity parameter, suggesting two diffusion modes. Fraction of the clusters that contribute to these diffusion modes is determined. A systematic study of dynamics of aqueous solutions of PEG is important in order to address different phenomena such as clustering of macromolecules that are observed in a biological cell. Strategies for modifying the model system is also discussed.

Why PFG NMR?

- Pulsed-field gradient (PFG) NMR is a technique that can provide a quantitative measure of molecular motion over the millisecond to second time scale.
- NMR offers simultaneous measurement of different species either by chemical shift or relaxation time.

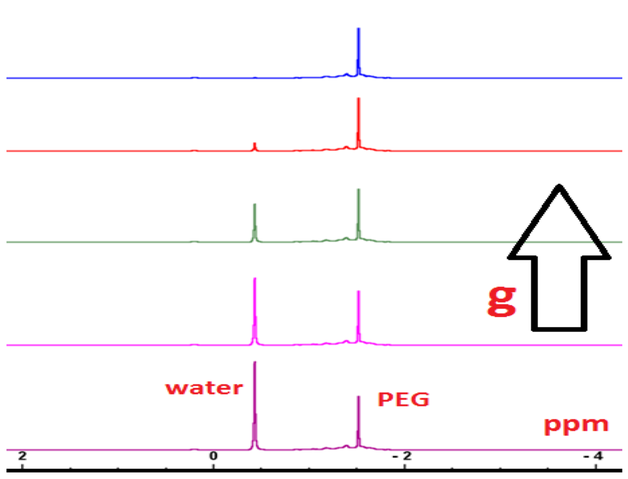
Spin Echo



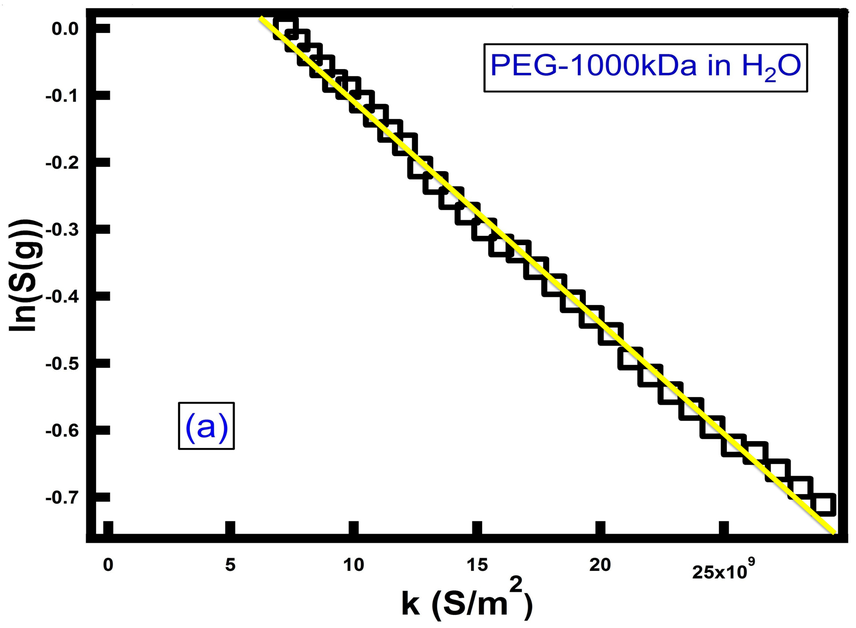
- First gradient dephases the signal.
- Second gradient rephases the signal.
- IF NO MOVEMENT during Δ : FULL signal recovered.
- IF MOVEMENT OCCURS during Δ: LOSS of signal.

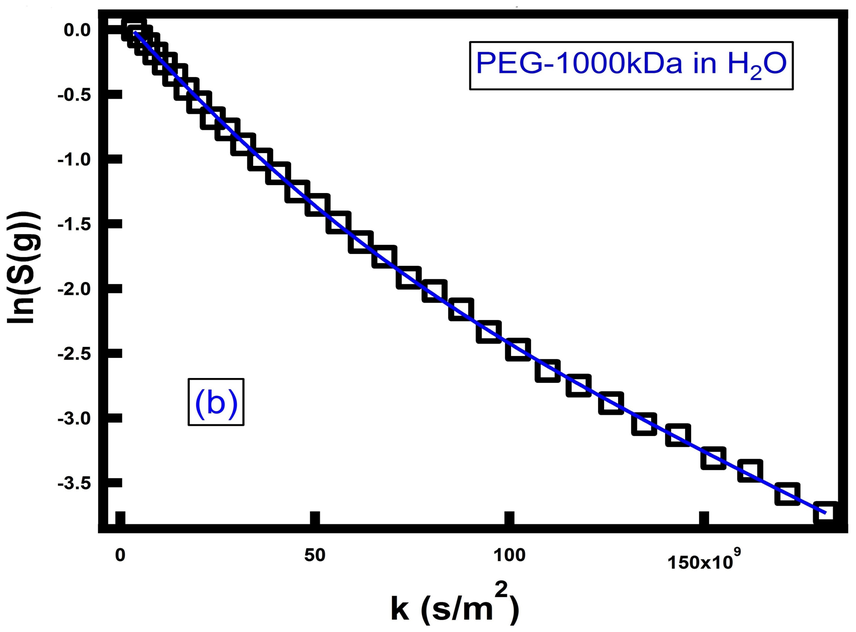
NMR Signal Attenuation

Diffusion profile is obtained by increasing magnitude of field gradient for repeated 1D experiments.



Decay of NMR signal : Aqueous Solution of PEG-1000 kDa





Mono exponential decay of signal (a) at lower field gradients (Solid yellow line is the fit to equation (1)) . A Bi-exponential (b) behaviour is observed when the applied field gradient range is increased (solid blue line is the fit equation (2)) .

Mono-exponential signal attenuation :

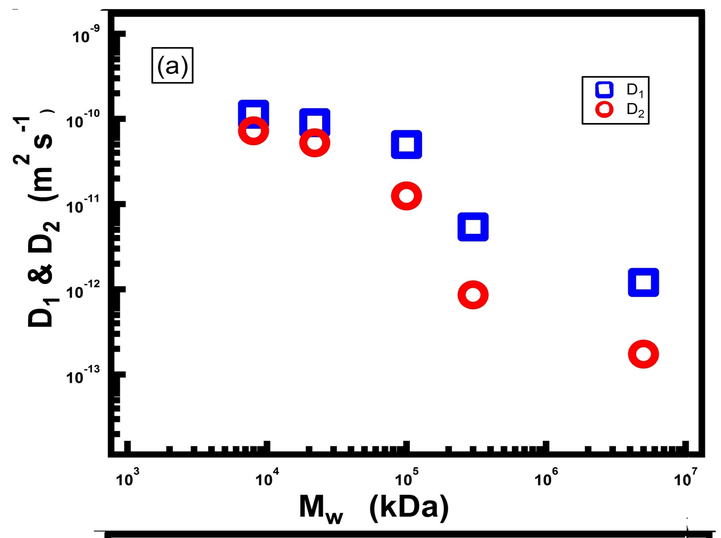
$$S(g) = S_0 \exp(-k D)) \quad \ldots\ldots\ldots\ldots\ldots (1)$$

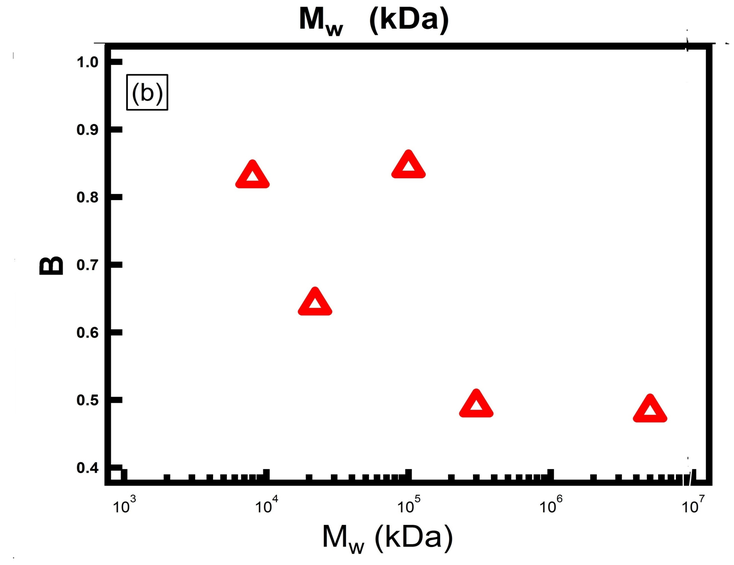
where $k = \gamma^2 g^2 \delta^2 (\Delta - \delta/3)$

Bi-exponential signal attenuation :

$$S(g) = B \exp(-kD1) + (1-B) \exp(-kD2) \quad \ldots\ldots\ldots (2)$$

Fast and Slow Diffusion Modes





Future Directions

- Examine PEG cluster formation over broad range of concentrations (including dilute regime).
- Extending the study to charged polymer in the presence of macromolecular crowding.
- Examine the role of sample homogenization.
- Study of diffusion of charged polymers in the presence of polydisperse crowder.

Acknowledgements

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Reference

[1] Palit, Swomitra, et al .Phys. Rev. Lett. (2017)

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