8TH PACIFIC RIM CONFERENCE ON RHEOLOGY, May 15-19, 2023

UNIVERSAL DIFFUSION OF DENDRIMERS IN SEMIDILUTE SOLUTIONS OF LINEAR POLYMERS

Silpa Mariya[1], Jeremy J. Barr[2], P. Sunthar[3] and J. Ravi Prakash[4]

[1] IITB-Monash Research Academy, Powai, Mumbai, 400076, India
[2] School of Biological Sciences, Monash University, Clayton, VIC 3800, Australia
[3] Department of Chemical Engineering, Indian Institute of Technology, Mumbai, 400076, India
[4] Department of Chemical and Biological Engineering, Monash University, Clayton, VIC 3800, Australia

ABSTRACT

Understanding the diffusion of nanoparticles and macromolecules in biopolymer networks is important for many biological and medical applications[1,2]. For example, elucidating the mechanisms underlying the transfer of macromolecular drugs into living tissue is essential for their use as drug delivery vehicles[3]. The role of the structure of the diffusing species as well as the polymer matrix in determining the physics of the diffusion process has been widely studied experimentally using probe species such as nanoparticles or branched polymers with well defined topologies in semidilute polymer solutions of linear polymer chains[4−7]. The results of these experimental studies have been described by hydrodynamic[8], scaling[9] and computational models[10], which have led to many insights identifying the key length and time scales involved. The theoretical models have however been confined to studying the diffusion of nanoparticles, which are hard spheres. The applicability of these models to situations when the probe diffusing species are soft tenuous particles such as a star polymers or dendrimers is currently unknown. In the present work, a multi-particle Brownian dynamics simulation algorithm, based on a modification of the GPU-accelerated python package HOOMD-blue[11], is used to describe the diffusion of dendrimers of arbitrary topology in a semidilute solution of linear chains. Diffusive and sub-diffusive regimes for the probe dendrimer and the background linear chains are identified and their dependence on the key parameters that determine length and time scales are elucidated. A new scaling law for dendrimer diffusivity as a function of the ratio of its mean size to the correlation length of the semidilute solution is proposed, which differs significantly from previously proposed scaling laws for hard sphere nanoparticles. With the appropriate choice of scaling variables, it is shown that data for dendrimers of different architectures can be collapsed onto a mater curve, independent of architecture. The Gaussian character of normalised particle displacements at various times, as a function of solution concentration, is also examined. It is shown that the central difference between dendrimers and hard sphere nanoparticles, which is responsible for the distinctness of their diffusive behaviours, is the reduction in the mean size of a dendrimer with increasing solution concentration.

REFERENCES

1. Salata, O. V. Applications of nanoparticles in biology and medicine, *Journal of nanobiotechnology*, **2(1)**, 1-6, 2004.

2. Rudramurthy, G. R., Swamy, M. K. Potential applications of engineered nanoparticles in medicine and biology: An update, *JBIC Journal of Biological Inorganic Chemistry*, **23**, 1185-1204, 2018.

3. Jain, R. K., Stylianopoulos, T. Delivering nanomedicine to solid tumors, *Nature reviews Clinical oncology*, **7(11)**, 653-664, 2010.

4. Cheng, Y., Prud'Homme, R. K., Thomas, J. L. Diffusion of mesoscopic probes in aqueous polymer solutions measured by fluorescence recovery after photobleaching, *Macromolecules*, **35(21)**,8111-8121, 2002.

5. de Kort, D. W., Rombouts, W. H., Hoeben, F. J., Janssen, H. M., Van As, H., van Duynhoven, J. P. Scaling behavior of dendritic nanoparticle mobility in semidilute polymer solutions, *Macromolecules*, **48(20)**,7585-7591, 2015.

6. Kalwarczyk, T., Ziebacz, N., Bielejewska, A., Zaboklicka, E., Koynov, K., Szymanski, J., ... , Hołyst, R. Comparative analysis of viscosity of complex liquids and cytoplasm of mammalian cells at the nanoscale, *Nano letters*, **11(5)**, 2157-2163, 2011.

7. Smith, M., Poling-Skutvik, R., Slim, A. H., Willson, R. C., Conrad, J. C. Dynamics of flexible viruses in polymer solutions, *Macromolecules*, **54(10)**, 4557-4563, 2021.

8. Cukier, R. I. Diffusion of Brownian spheres in semidilute polymer solutions, *Macromolecules*, **17(2)**, 252-255, 1984.

9. Cai, L. H., Panyukov, S., Rubinstein, M. Mobility of nonsticky nanoparticles in polymer liquids, *Macromolecules*, **44(19)**, 7853-7863, 2011.

10. Chen, A., Zhao, N., Hou, Z. The effect of hydrodynamic interactions on nanoparticle diffusion in polymer solutions: a multiparticle collision dynamics study, *Soft matter*, **13(45)**, 8625-8635, 2017.

11. Anderson, J. A., Glaser, J., Glotzer, S. C., HOOMD-blue: A Python package for high-performance molecular dynamics and hard particle Monte Carlo simulations, *Computational Materials Science*, **173**, 109363, 2020.