

SHEAR INDUCED ADSORPTION OF POLYMER ONTO NEUTRAL SURFACES

VENKAT BALA & DR. COLIN DENNISTON, THE UNIVERSITY OF WESTERN ONTARIO, CANADA, VBALASU8@UWO.CA

INTRODUCTION

Experiments involving the protein VWF (von Willebrand factor), present in our blood have shown its importance in preventing blood loss under high shear stress conditions. Elevated shear levels found during blood loss activate this protein's adhesion potential causing it to stick to walls for blood platelets to adhere.



http://medimoon.com/2013/12/new-drug-trettenapproved-by-fda-to-prevent-bleeding-in-rare-clottingdisorder/

The unusually large size of this multimeric protein, 2050 amino acids/monomer and lengths reaching up to $\approx 100 \mu m$ are attributed as reasons as to why this counter-intuitive phenomena occurs.

METHOD

- MD simulations with full hydrodynamic interactions were carried out using LAMMPS/USER-LB package with nanoscale units ([1],[4])
- 12-6 *lj/cut* repulsive potential was used to model excluded volume interactions between monomers with $\epsilon = 4.14195, \sigma = 1.5 \text{ and } r_c = 2^{1/6} \sigma$
- Polymer was composed of 96 monomers, each enveloped within a spherical shell consisting of 30 atoms interacting with the thermal lb/fluid bath



- Chain held together by Finitely Extensible Non-linear Elastic (FENE) bonds
- 12-6 *lj/cut* potential used for the attractive interaction between the polymer and wall atoms, with $\sigma = 1.5$ and $r_c = 2.5\sigma$
- Interaction strength varied, $\epsilon_w = 0.045, 0.055, 0.065, 0.075, 0.085, 0.095$

RESULTS

• Thermal fluctuations cause small protrusions into the bulk, which get pulled by the shear and unfold the polymer causing it to stick to the wall. This creates an immobilized grid to which blood platelets adhere causing the blood to clot



• Characterizing adhesion by counting the number of contact points along the chain, M within half the cut-off distance of the polymer-wall attractive potential, i.e $r_z < r_c = 2.5\sigma$



Contact parameter (steady state time-averaged) as a function of shear for various adhesion strengths ϵ_w . Here $\tau = a^2/(\mu_0 k_B T)$, μ_0 being the Stokes mobility, is the single monomer diffusion time

• Cumulative probability distribution of the net force acting on the polymer in the *z* direction



- case
- Difference quite small
- bead HI



– Results for $\epsilon_w = 0.095$, $\dot{\gamma}/\tau = 0.5$. Higher probability for F_z to be negative for the larger monomer

- Need sufficiently high number of terms in a multipole expansion to properly account for the bead-

DISCUSSION

- Recent works using Brownian dynamics simulations, unable to observe shear induced adsorption with HI [2]
- In the bulk, polymer gets stretched out \rightarrow dramatic loss of conformational entropy, adhered state to the wall preferred!
- Particle size effects, Stoke's flow equations \rightarrow LINEAR. Green's function solution satisfying no-slip condition at a plane wall \rightarrow Blake tensor, μ^B

$$abla p(\mathbf{r}) - \eta \,
abla^2 \mathbf{v}(\mathbf{r}) = \mathbf{f}(\mathbf{r}), \quad
abla \cdot \mathbf{v}$$

• Hydrodynamic interactions between spheres of radii *a* located at **r**, **r**', no shear, [3]

$$\mu(\mathbf{r}, \mathbf{r'}) = \left(1 + \frac{a^2}{6} \nabla_{\mathbf{r}}^2 + \frac{a^2}{6} \nabla_{\mathbf{r'}}^2\right) \mu$$

- Higher order terms in the multipole expansion could possibly yield correct dynamics near wall
- Effect of external shear flow on the HI tensor must be taken into account



REFERENCES

- [1] S. Plimpton, J. Comput. Phys., 117 (1995), pp. 1-19
- [2] M. Radtke, M. Radtke, and R. Netz, Eur. Phys. J. E, vol. 37, no. 3, 2014
- S. W. Schneider, S. Nuschele, a Wixforth, C. Gorze-[3] lanny, a Alexander-Katz, R. R. Netz, and M. F. Schneider, Proc. Natl. Acad. Sci. U. S. A., vol. 104, no. 19, pp. 7899-7903, 2007
- [4] F. E. Mackay, S. T. T. Ollila, and C. Denniston, Comput. Phys. Commun., vol. 184, no. 8, pp. 2021-2031, 2013