

Supporting Information

Brownian dynamics simulations of polymer - latex suspensions under steady shear

Sriram Krishnamurthy,¹ Gopal Parthasarathy,² Ronald G. Larson² and Ethayaraja Mani^{1*}

¹Polymer Engineering and Colloid Science Lab, Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai 600036, India

²Department of Chemical Engineering, University of Michigan, Ann Arbor, Michigan 48109, United States

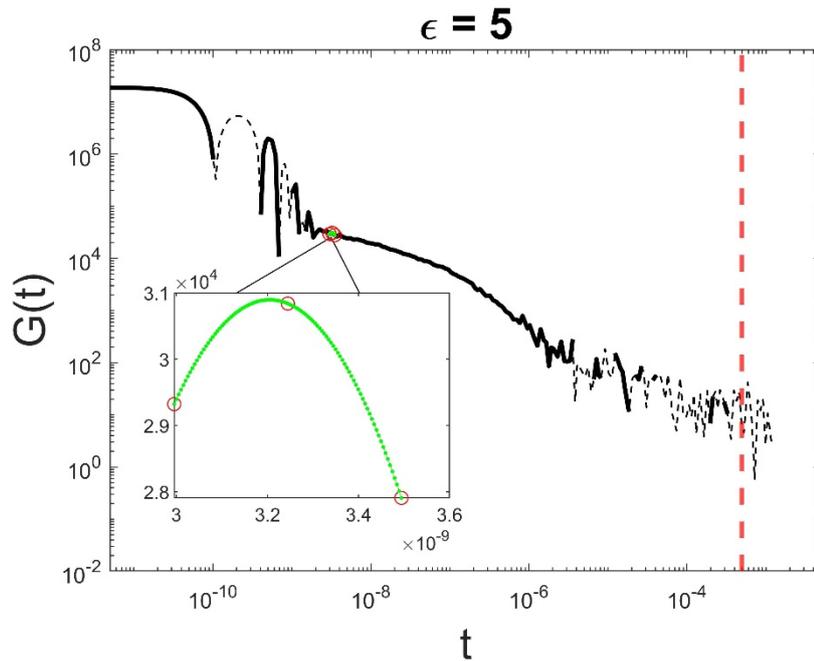


Figure S1: A sample curve for $G(t)$ for $\epsilon = 5$, 40 dumbbells/particle, 8 particles. The solid line corresponds to the simulation data. The dashed lines are absolute values of negative values which at early times are due to inertial “ringing” or oscillation of beads or particles in attractive potential wells, and at long time are the result of noise. The red vertical dashed line is the noise-related cut-off value that we get from the integration procedure mentioned in the main text and Figure S2. Inset shows 100 Interpolated points (small green dots) between the simulation data (red circles) using a smooth spline method (using the Matlab[®] in-built function *interp1*).

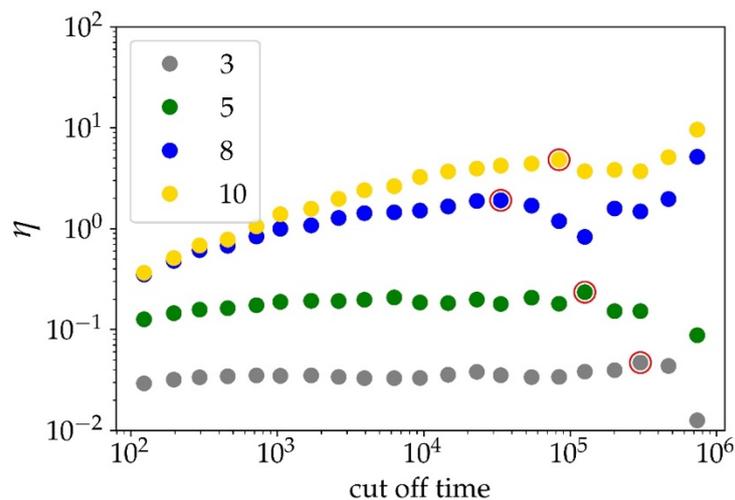


Figure S2: Sample curves for viscosity calculation. This curve shows the values of viscosity calculated from integrating $G(t)$ for different values of the cutoff times. At longer cut-off times, we chose the highest value (marked in red circle) after which successive calculations show a decrease in viscosity. Beyond this cut-off, $G(t)$ becomes very noisy and those points are then neglected in the calculation of viscosity.

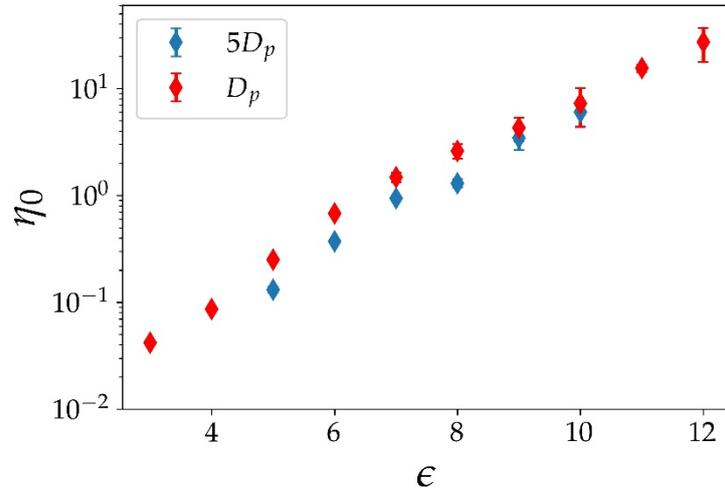


Figure S3. Zero-shear viscosity as a function of sticker strength (ϵ) for $D_p = 0.057 \frac{a^2}{\tau_0}$ and $D_p = 5 \times 0.057 \frac{a^2}{\tau_0}$.

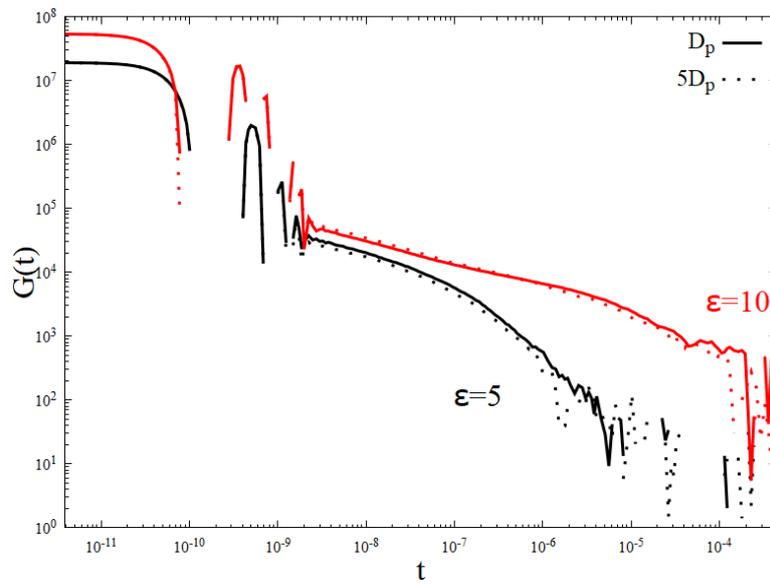


Figure S4. Comparison of $G(t)$ for D_p and $5D_p$ for different ϵ values.

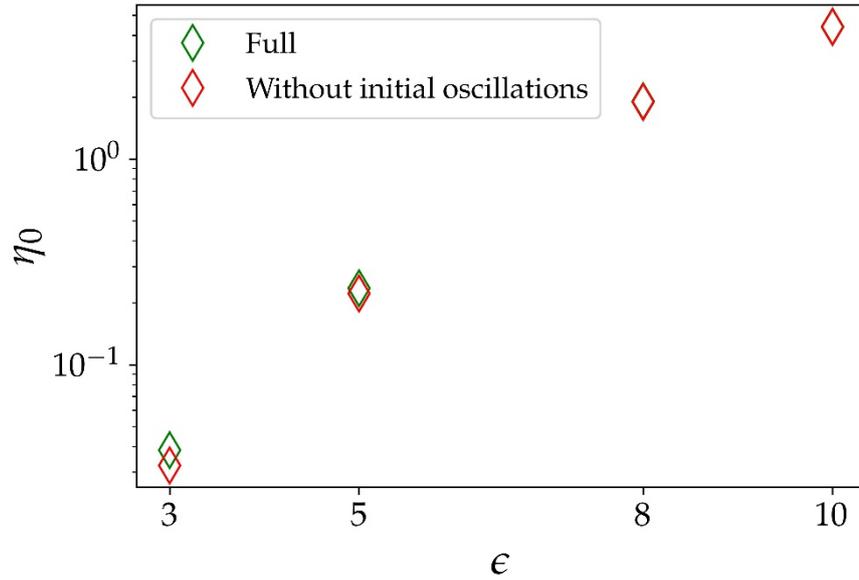


Figure S5: Comparison of zero-shear viscosity calculated with and without the initial oscillatory phase in the SACF.

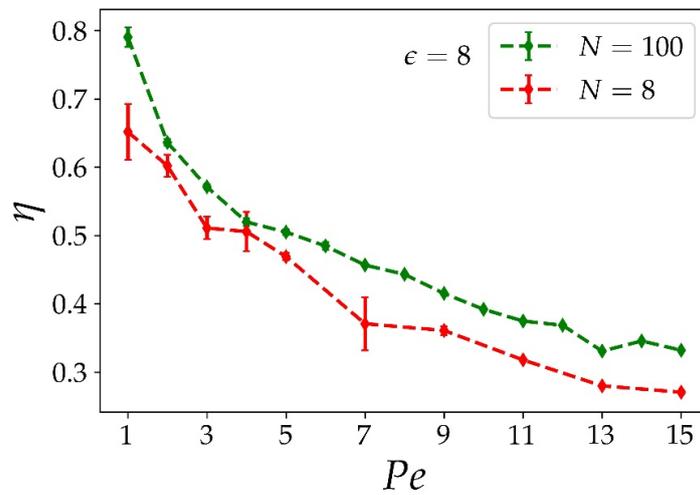


Figure S6: viscosity vs Pe for different number of particles (N_p) with 40 polymers per particle

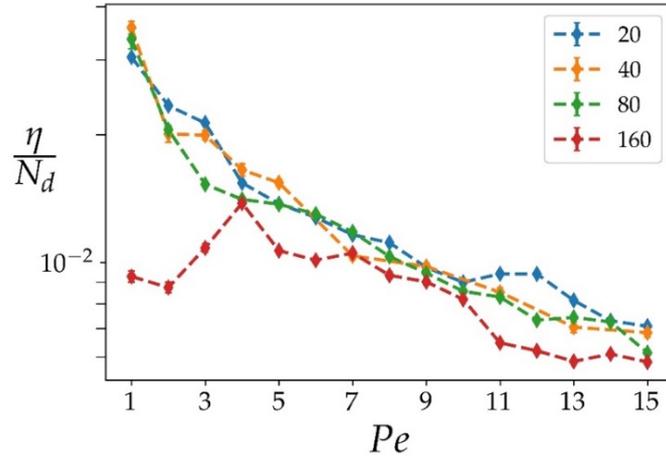


Figure S7: Scaled viscosity (i.e., viscosity per dumbbell) as a function of shear rate for different concentration of dumbbells. All the simulations were performed for $\epsilon=10$.

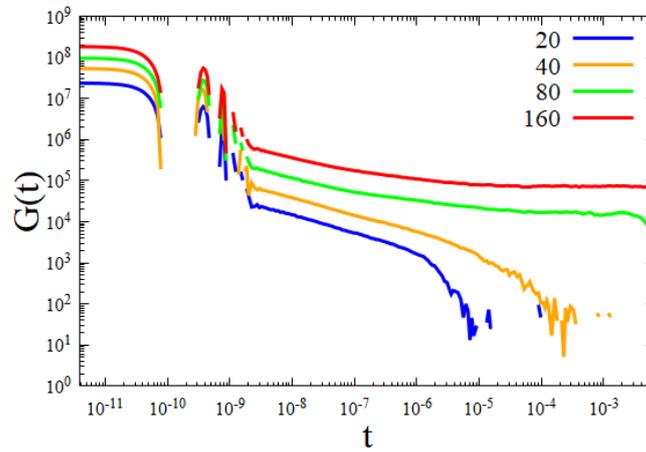


Figure S8. Stress relaxation modulus $G(t)$ for different number of dumbbells per particle (N_d) at $\epsilon = 8k_B T$. Modulus and time are in dimensionless units of $[k_B T/a^3]$ and τ_0 , respectively.

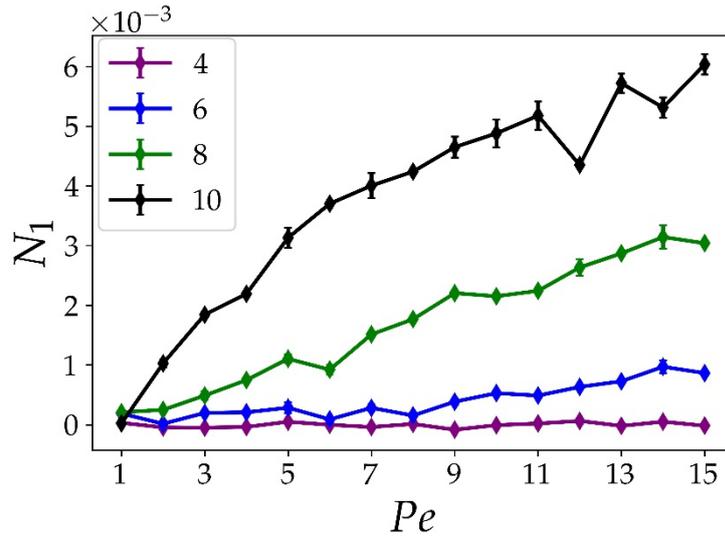


Figure S9: First normal stress difference (N_1) as a function of Pe for different ϵ values for the dumbbell model

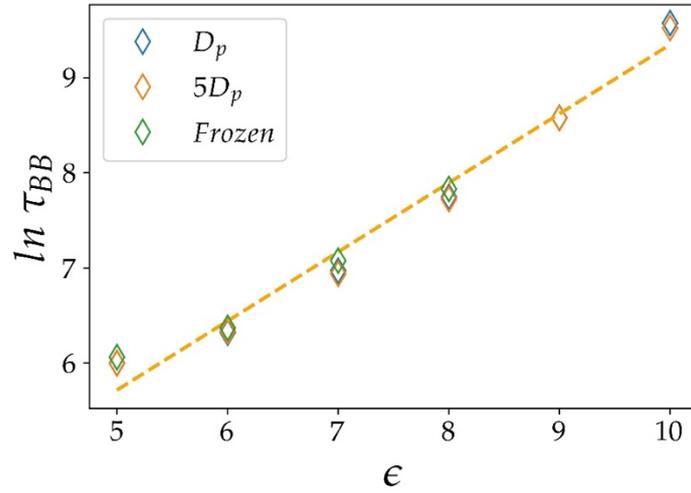


Figure S10: Bridge-to-Bridge (τ_{BB}) transition times as a function of ϵ .

Table S1 : Zero-shear τ_{BL} and τ_{LB} (in the units of τ_0) as functions of ϵ for i) frozen colloids and ii) colloids with diffusivity increased five-fold.

ϵ	$\ln \tau_{LB}$		$\ln \tau_{BL}$	
	Frozen	$5D_p$	Frozen	$5D_p$
5	6.78	6.73	5.22	5.20
6	7.08	7.08	5.67	5.65
7	7.81	7.73	6.35	6.34
8	8.58	8.53	7.17	7.14
9	-	9.36	-	8.00
10	-	10.18	-	8.88