Supporting Information: Nano-Pump based on Exothermic Surface Reactions

November 11, 2020

1 Extrapolation to water viscosity

In order to estimate the flow of an aqueous solvent, we must map the DPD results to fluid with the viscosity of water. This requires re-scaling the flow velocity, as the viscosity of the DPD model proposed by Groot and Warren [1] is ~ 20 times smaller than that of water, when expressed in the same units. In the Stokes regime, the the flow velocity is inversely proportional to the viscosity. Such a dependence is indeed observed in Fig. 1.

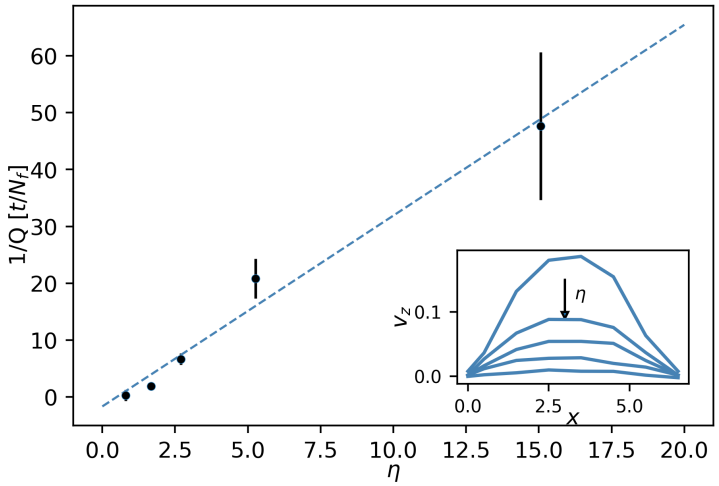

Figure 1: Inverse flow rate as function of computed viscosity through Poiseuille flow and its linear fit (dashed line). The inset shows the z-velocity profiles along the x-direction. Simulations carried at higher viscosities were carried out by changing γ and with r_c equals 1.2 instead of 1.0 to achieve high viscosity with moderate values of γ.

We estimated the viscosity of the DPD fluid by carrying out simulations of Poiseuille flow in a cylinder resulting from the application of a constant force per particle of $0.03N$ in the z direction. We vary η by changing γ and r_c. The viscosity of the DPD fluid is estimated, assuming Poiseuille flow, in which case using $\eta = \rho f_z R^2/(4v_{max})$.

2 Pump Wall

The pump-wall consists of 'frozen' DPD particles at a (high) reduced density of ~ 45, thereby mimicking a smooth and non-penetrable surface. To reproduce non-slip boundaries, we added a sinusoidal, longitudinal corrugation to the cylinder surface with an amplitude of 1/4 in reduced units and a period of $\pi/2$. We verified that this corrugation made the flow velocity vanish (less than 5% from the maximum velocity) close to the wall in a body-force-driven flow through a cylinder. Alternatively, we can suppress friction with the wall (slip boundary conditions) by smoothing the boundaries.

The wall could be made to act as a thermostat, by applying dissipative and random forces between wall and fluid particle with $\gamma_{solid} = 10 \cdot \gamma$. Depending on the geometry of the constriction in the channel, the thermalised case resulted in 25%-50% lower flow rate compared to the pure repulsive wall ($\gamma_{solid} = 0$). For instance, Fig. 2 shows the flow as a function of the thermalisation coefficient (γ_{solid}) in the case of a non-slip wall. We find that the wall absorbs most energy on the the active region, where reactions happens. Thermalising the cylindrical wall has a minor effect on the flow. We stress that our model for reaction and flow at a solid-liquid interface is highly simplified: however, to obtain a more realistic description would require fully atomistic simulations of the reaction dynamics and flow at a specific interface. As we are interested in generic effects, such simulations were beyond the scope of the present study.

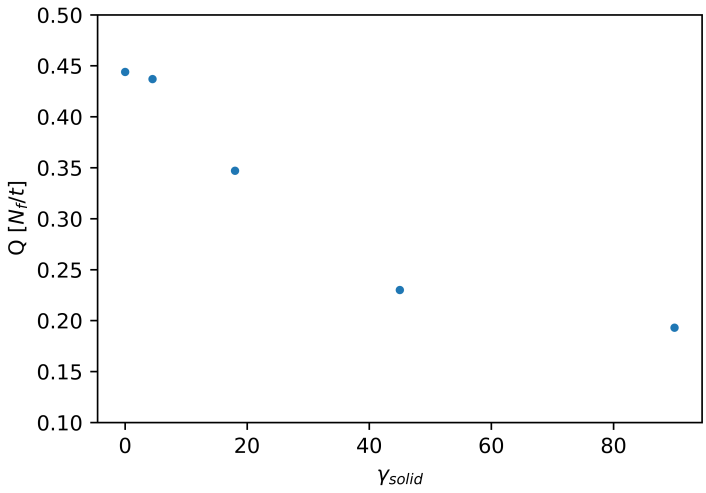

Figure 2: Flow as function of γ_{solid} for non-slip wall and a reaction rate f=1. In the simulations, we used a higher rate f=10, and rescaled the results back to f=1. Energy of reaction is assumed to be 1eV.

All DPD calculations were carried out using the HOOMD-blue [2] DPD code.

The remainder of the code was written in PyCUDA.

References

[1] Groot, R. D. and Warren, P. B. *Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation* J. Chem. Phys.,11,4423–4435, 1997.

[2] Phillips, C. L, Anderson, J. A., and Glotzer, S. C. *Pseudo-random number generation for Brownian Dynamics and Dissipative Particle Dynamics simulations on GPU* devices, J. Comp. Phys. 230 7191–7201, 2011.