Motion of particles driven through a polymeric network

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Background: use of face mask widespread after the pandemic.

Reason for facemask use: Stop airborne respiratory micro-droplets particles

Image source: google

Features to be considered:

1. WHO guideline of mask :
Three layer mask **Outer + middle layer** : hydrophobic material like polypropylene;
Inner layer : Hydrophilic like cotton

2. Breathability denoted by pressure drop. Average pressure drop 2 Pa order at respiration rates at rest (~35 L/min) velocity airflow.

Challenge: Designing efficient face mask ensuring normal breathability

Goal:
Understand droplet movement inside facemask in presence of pressure difference and increased efficiency of facemask by tuning different network properties.

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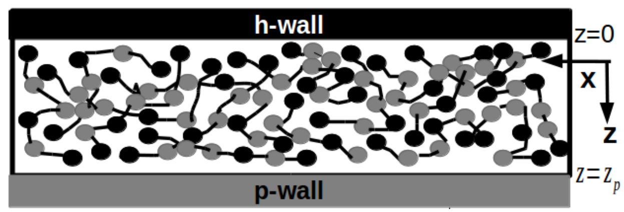
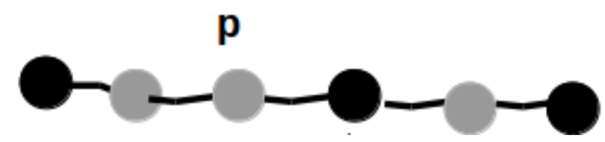
Model

Air and moth-cavity two different environment
Polymer network. Droplet: tracer colloid particle (TCP)

Prepare interpenetrating polymeric network confined between asymmetric wall

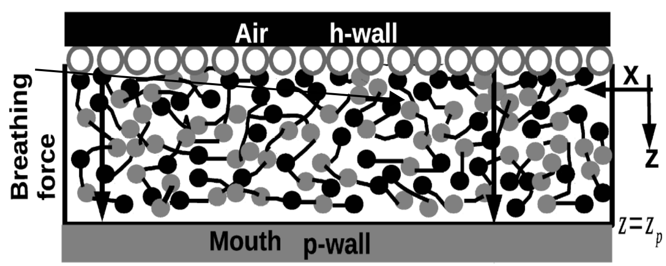




$$\sigma = 1 \mu m$$

High pressure

Droplets as TCP; interaction with both beads



$$\epsilon_{tr,p} > \epsilon_{tr,h}$$

$$F = F_0(1 - z/z_p)$$

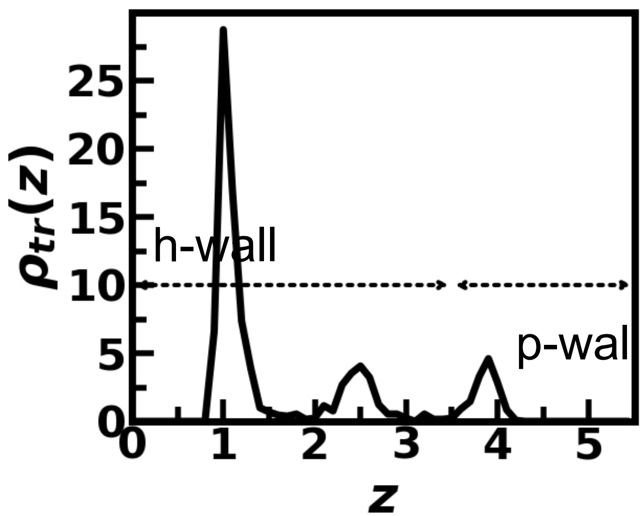
Low pressure

Simulation scheme:

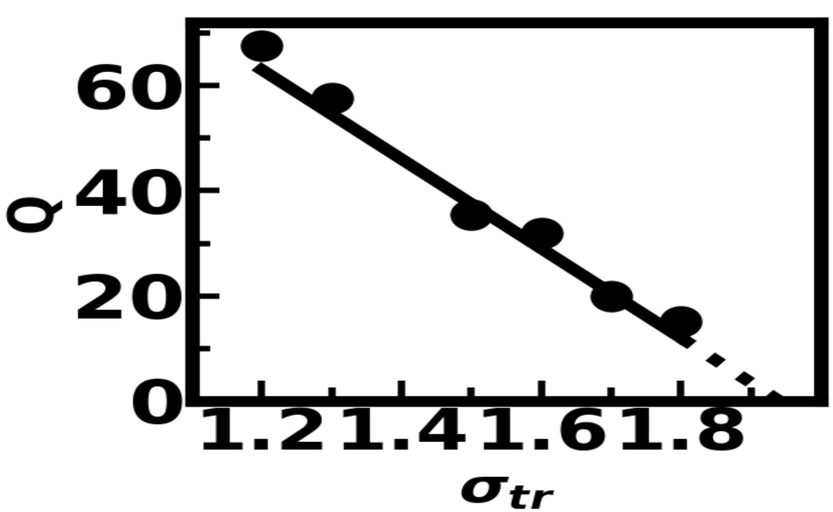
- Perform Langevin dynamics in NVT using LAMMPS
- **Calculate density profile of TCP**

Results

$$F_0 = 0$$



Density profile of TCP along confinement direction

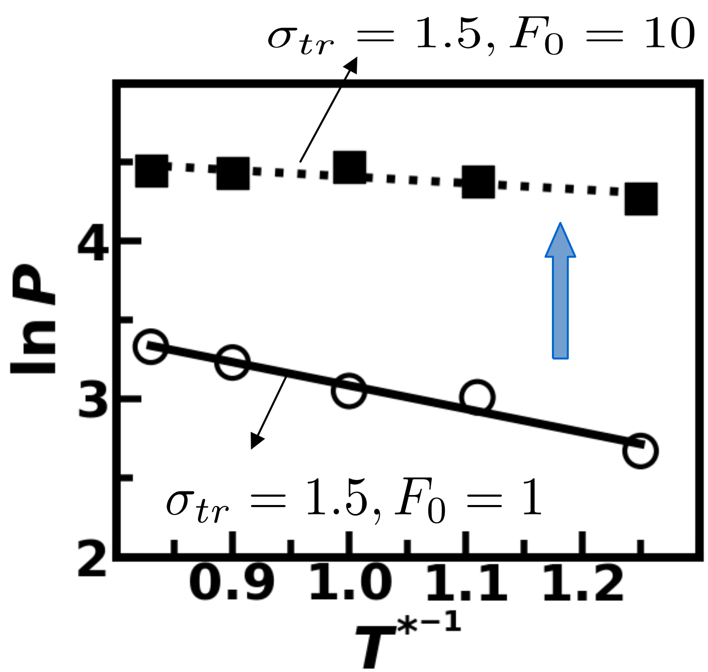


Q=Particles reaching P wall;
integrating density profile close to the wall

Results

Temperature effect

P=100-Q



- $\ln P \sim T^{*-1}$
- $P \sim e^{-F_B T^{*-1}}$
- Arrhenius behaviour
- TCP motion is an activated process.
- Slope F_B is barrier hegiht.
- F_B decreasing with driving force.

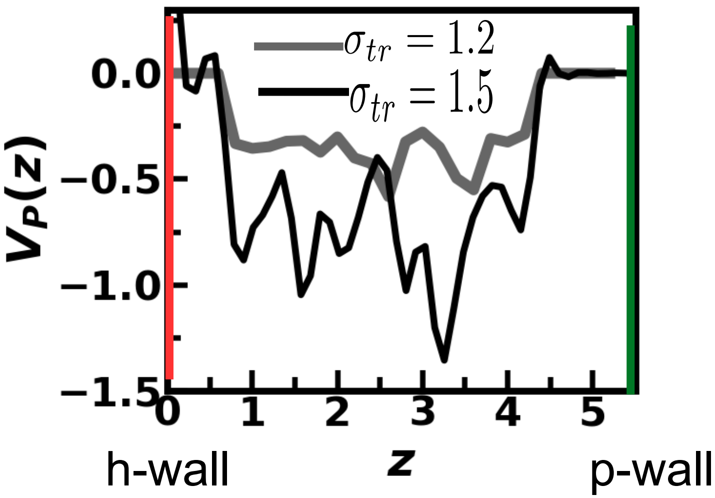
Results

Potential energy profile along the z direction per TCP particle

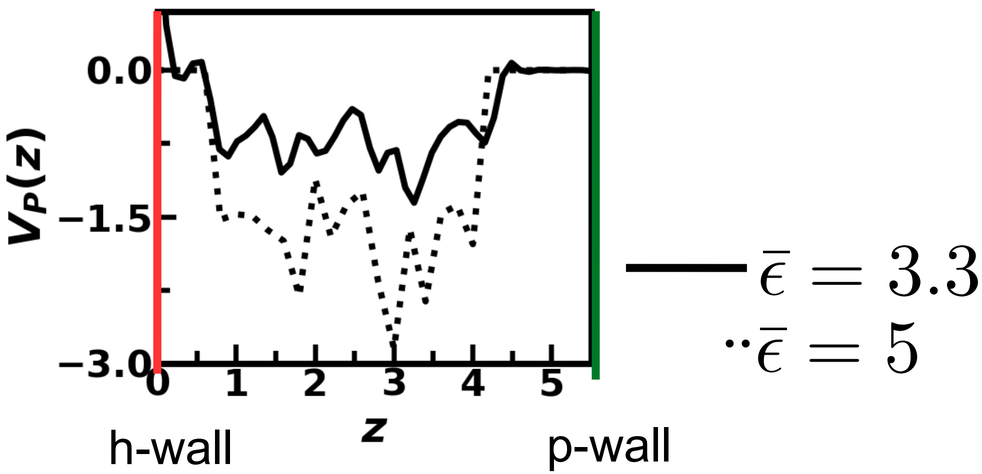
- $V(z) = V_P(z) + V_H(z)$

$$\bar{\epsilon} = \frac{\epsilon_{tr,p}}{\epsilon_{tr,h}}$$

$F_0 = 1 \quad \bar{\epsilon} = 3.3$



$\sigma_{tr} = 1.5 \quad F_0 = 1$



Larger TCP face large barrier

Large $\bar{\epsilon}$ tends to localize the TCPs inside network

Barrier can be tuned with tuning network properties

Parameter space

- Composition h:p
- Tracer bead interaction $\bar{\epsilon}$
- Rigidity $k_b = k_\theta = k$
- Confinement length z_p

Summary:

Increase mask efficiency using different network parameters

Room temperature, $\sigma_{tr} = 1.5, F_0 = 1$, $\Delta P \sim 1Pa$

To achieve e>90% from our model:

2) h:p = 50:50

3) $\bar{\epsilon} \geq 3.3$

4) rigidity k > 200

5) $z_P = 5.5 \mu m$

Thank you