Model studies on motion of respiratory droplets driven through a face mask

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Abstract – Face masks are used to intercept respiratory droplets to prevent spreading of airborne diseases. Designing face masks with better efficiency needs microscopic understanding on how respiratory droplets move through a mask. Here we study a simple model on the interception of droplets by a face mask. The mask is treated as a polymeric network in an asymmetric confinement, while the droplet is taken as a micrometer-sized tracer colloidal particle, subject to driving force that mimics the breathing. We study numerically, using the Langevin dynamics, the tracer particle permeation through the polymeric network. We show that the permeation is an activated process following an Arrhenius dependence on temperature. The potential energy profile responsible for the activation process increases with tracer size, tracer bead interaction, network rigidity and decreases with the driving force and confinement length. A deeper energy barrier led to better efficiency to intercept the tracer particles of a given size in the presence of driving force at room temperature. Our studies may help to design masks with better efficiency.

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Using a face mask (FM) has been commonplace much beyond the usual medical purpose [1], since the COVID-19 pandemic. The World Health Organization (WHO) mandates the use of FM to prevent the spread of COVID-19 [2]. By now it is established [3–5] that the SARS-COV-2 virus responsible for COVID-19 is air-borne, like many other air-borne diseases, namely, tuberculosis, pneumonia and so forth. FM is the simplest measure to prevent spreading of any air-borne disease [4,6,7] by intercepting respiratory droplets of micrometer size, emitted when an affected person talks, sneezes or coughs. Respiratory micro-droplet propagation through air has been intensively studied [6,8–11]. However, relatively much less is known about micro-droplet movement through a FM.

FMs are typically made of fabric materials of entangled polymeric networks [3], which allow essential molecules to be exchanged with the atmosphere and the human body but stop the movement of larger particles [3,12]. Normal N95 FMs with fibres are commercially used. There are several layers in these FMs. The fibre diameter of filtration layer is about a few micrometers [13–16] with volume fraction typically less than 30% [13]. They capture 95% of the micro-droplets. The micro-droplets larger than the mean pore size are stopped due to geometrical constraints. The smaller micro-droplets are captured through interception, diffusion, and electrostatic attraction [5,14,17]. Such capture is the essence of a FM. But they show reduction in efficiency in humid conditions due to charge loss [18]. In the search for stable FM performances, different possibilities are explored which include, for instance, using tribo-electric generators [5,19,20], mixture of fabrics with different compositions [12], and multiple layers [21]. Nanofibres [17] and metal-organic framework filters [22,23] are shown to be a promising route for better FMs. However, they are plagued with breathing difficulty due to pores of nano-meter sizes. Reduction of leakage through FMs is also necessary for better efficiency [24].

Given this backdrop, theoretical understanding of various aspects of a FM network to control the efficiency of intercepting micro-droplets would be highly imperative. A numerical study using the continuum fluid dynamics equations suggests that the droplet movement is a combined effect of capillary action and breathing force inside the FM [25]. At a more microscopic level, one may consider the respiratory droplets as colloidal particles moving through a porous polymeric network structure. Particle movement through a polymer network has

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been widely studied [26–31] due to its importance in intracellular transport, fluid rheology, materials engineering and so forth. It is reported that polymer networks are typically viscoelastic and heterogeneous in nature and this affects tracer movement [27] leading to non-Gaussian displacement distribution and sub-diffusivity [31]. It is also observed that the movement can be tuned with different network properties like network rigidity, binding affinity of tracer with network and tracer size [26]. Higher rigidity and affinity result in slower motion or caging behavior for tracer movement inside polymer network. Polymer mobility also affects the tracer movement compared to a frozen polymer network [31].

In the case of a FM there are a few important aspects: 1) The WHO recommends that masks should be made up of three layers [21,32]: a polar material like cotton layer inside towards mouth and a hydrophobic material in the middle and the outermost layers [5,32,33]. 2) The penetration of the droplet inside the porous mask also depends on the wettability of the fabric materials by the micro-droplets [34]. 3) It is necessary to consider breath-ability, an indicator of resistance to airflow by the mask while breathing and given in terms of the pressure drop inside the mask during airflow [12]. The average pressure difference in normal breathing is found to be around 2.5 ± 0.4 Pa [12]. We study a model to understand these aspects at a qualitative level. A schematic of the model is shown in fig. 1. The FM is modelled in terms of a network of polymeric strands with two different kinds of beads of micrometer size [13]. The beads have low volume fraction so that there is sufficiently large void spaces (nearly 80%) [13] to allow exchange of small molecules easily. One class of beads (h-beads) are taken to mutually interact more strongly than the other class of beads (p-beads). The h-beads mimic hydrophobic species those are known to collapse [35–37] and ensure a strong interpenetration of the network. The network is under an asymmetric h (black) and p (grey) wall. The polymer consists of two beads: h-beads are shown as solid black circles and p-beads are shown as solid grey circles. h-beads prefer h-wall and p-beads prefer p-wall. Tracers particles (hatched open black circles) are added close to the h-wall. Tracers prefer p-beads and p-wall. Force on each tracer particle (mimic breathing) is added from h-wall to p-wall. Forces are represented by black arrows from h-wall to p-wall. The force is maximum at z = 0 and zero at z = zp. (The y-axis is pointing into the page.)

We study the motion of the polymeric beads and the TCPs using the Langevin dynamics simulations [38]. The equation of motion consists of the inertial term, the interaction forces, the drag force due to the medium and drive force only on the TCPs. In the case of polymeric beads, we consider the force arising from the elasticity but ignore the drive force compared to the elastic force. It may be noted that in this description, the dispersing medium is not considered explicitly, but taken in terms of drag force. The volume fraction of the TCPs (~ 26%) is also low as that for the polymeric beads (~ 21%), so that we ignore the hydrodynamic forces for the beads and TCPs. Let us consider the movement of the TCPs from h-wall to p-wall. The fraction of tracer particles reaching the p-wall is the permeation P through the mask, while the efficiency of the mask is e = 100 − P. We find that the permeation of the TCPs is an activated process, the energy landscape responsible for the activated process being governed by the TCP and p-bead interaction. A large activation barrier leads to a lower P and hence, larger e. We study the efficiency of intercepting the TCPs, fixing size, the driving force and the ambient temperature while varying the composition of the polymeric strands, TCP interaction with the p-beads, network rigidity and confinement size. We find that a 50:50 mixture of polymeric beads and stronger TCP and p-bead interaction gives better efficiency. Mask efficiency linearly increases with increasing network rigidity and with decreasing confinement size. These may be helpful to design a mask with large efficiency ensuring normal breath-ability condition.

**Model and simulation.** – Each polymeric strand is composed of two kinds of beads of the same diameter σ and mass m in a given h:p ratio, randomly distributed over the strand. The non-bonded interaction between two monomers is taken through the Lennard-Jones (L-J) 12-6 potential: $V_{\alpha\beta}(r_{ij}) = 4\epsilon_{\alpha\beta}[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^6]$, $r_{ij} < 3\sigma$. 

![Fig. 1: A model diagram of a polymeric network confined in asymmetric h (black) and p (grey) wall.](Image 316x682 to 532x757)
Here $\alpha (= h, p)$ and $\beta (= h, p)$ stand for the bead types and $r_{ij}$ is the separation between two beads. $\epsilon_{\alpha\beta}$ is the strength of interaction and $\sigma$ the diameter of the beads. We take $\sigma$ the same for all other interactions. The bonded interaction corresponds to stretching between two neighbouring beads: $V_{\text{bond}}(r_{ij}) = \frac{1}{2}k_b(r_{ij}-r_0)^2$, where $r_0$ is the distance between neighbouring monomers and $k_b = 1.5\sigma$ is the equilibrium distance between monomers and $k_b$ the force constant. The change in bond angle costs energy: $V_{\text{angle}}(\theta) = \frac{1}{2}k_\theta(\theta-\theta_0)^2$, where $k_\theta$ is the force constant and $\theta = \cos^{-1}(\frac{r_{ij}^2+r_{jk}^2-r_{ki}^2}{2r_{ij}r_{jk}})$ is the angle produced by three consecutive monomers $i, j, k$ and $\theta_0$ is equilibrium angle, set to 114 degrees [39]. We consider a rigid network where the elastic deformation of any kind costs a lot of energy and ignore the distinction between these two elastic constants. Thus, we take $k_b = k_\theta = k$ to reduce the number of variables.

We place the polymeric system within two walls: The h-wall interacts with a particle via the L-J $9-3$ potential $V_{\text{f,wh}}(z_i) = \epsilon_{\text{f,wh}}\left(\frac{\sigma}{|z_i|}\right)^9 - \left(\frac{\sigma}{z_i}\right)^3$. Similarly, the p-wall interacts with a particle $V_{\text{f,wp}}(z_i) = \epsilon_{\text{f,wp}}\left(\frac{\sigma}{|z_i|}\right)^9 - \left(\frac{\sigma}{z_i}\right)^3$. Here $f = (h, p)$ stands for the bead type and $z_i$ is the $z$-coordinate of the $i$-th particle. The $\alpha$ values for all the interactions are taken to be the same but $\epsilon_{\text{h,wh}} > \epsilon_{\text{p,wh}}$ and $\epsilon_{\text{p,wp}} > \epsilon_{\text{h,wp}}$.

The TCPs interact with each other with strength $\epsilon_{\text{tr,tr}}$. The strength are $\epsilon_{\text{tr,h}}$ and $\epsilon_{\text{tr,p}}$ for the interaction of TCPs with $h$ and $p$ beads. They interact with two walls through the L-J $9-3$ potential with parameters $\epsilon_{\text{tr,wh}}$ and $\epsilon_{\text{tr,wp}}$ for $h$ and $p$ walls, respectively. We choose them to interact more favourably with the p-beads and the h-wall than the h-beads and the h-wall, respectively, so that $\epsilon_{\text{tr,wp}} > \epsilon_{\text{tr,wh}}$. We further take force over a TCP, $F(z) = F_0(1 - z/z_p)$.

We take $\epsilon_{\text{hh}}$ as unit of energy. The unit of mass is the mass of water of density $1 \text{ g/cm}^3$ in a sphere of diameter $1 \mu\text{m}$. The bead diameter ($\sigma = 1 \mu\text{m}$) [13-16] is the unit of length. We set dimensionless $\epsilon_{\text{pp}} = 0.33$ (1/3 of $\epsilon_{\text{hh}}$) while the cross-interaction between $h$ and $p$ monomers is taken to follow the Berthelot mixing rule. We set dimensionless wall particle interactions, $\epsilon_{\text{h,wh}} = 1.0$, $\epsilon_{\text{p,wh}} = 0.033$, $\epsilon_{\text{p,wp}} = 0.33$ and $\epsilon_{\text{h,wp}} = 0.033$. For these choices of the interaction parameters, the polymeric network is uniformly spread throughout the gap between two walls as shown in fig. S1 of the Supplementary Material Supplementarymaterial.pdf (SM). The dimensionless L-J energy parameters for TCPs are $\epsilon_{\text{tr,tr}} = 1.0$, $\epsilon_{\text{tr,wh}} = 0.033$, $\epsilon_{\text{tr,wp}} = 1.0$. The mass of the polymeric bead particles is taken to be that for water droplet of diameter $\sigma$. Similarly, the mass of the tracer particles is that for a water droplet of diameter $\sigma_{tr}$. We vary several parameters: $\bar{\epsilon} = \epsilon_{tr,h}/\epsilon_{tr,wh}$, the network rigidity $k$ and the confining length $z_p$. We perform simulations for various reduced temperature $T^* = \frac{\bar{\epsilon}k_BT}{\epsilon_{\text{hh}}}$.

The particle dynamics are computed via the underdamped Langevin equation of motion of the $i$-th particle with mass $m_i$ at position $\vec{r}_i(t)$ at time $t$:

$$m_i\frac{d^2\vec{r}_i}{dt^2} = -\zeta_i \frac{d\vec{r}_i}{dt} - \nabla \sum_j V^i(\vec{r}_i^a - \vec{r}_j^a) + \vec{F}_i^a + \vec{F}_I^\alpha,$$

(1)

where $\alpha$ is the particle type. $\alpha$ can stand for either the polymer beads or the TCP. $\zeta^\alpha$ is the friction coefficient. $V^i$ is the sum of all the relevant interactions for a given particle type. For the network beads, we consider bonded and non-bonded interactions with other network beads, TCPs and the walls and set $\vec{F}_I^\alpha = 0$. For TCPs we consider the interaction with other TCPs, network beads, the wall and in addition the external force, $\vec{F}_I$. The components of $\vec{F}_I^\alpha(t)$ are the Gaussian white noise with zero mean and variance, $6\zeta^\alpha k_BT(\bar{\epsilon} - \bar{\epsilon})$, where $k_B$ is the Boltzmann constant, and $T$ the temperature. Here $\zeta^\alpha = m_i^\alpha \gamma$, where $\gamma$ is the damping term due to friction of the network.

We perform simulation using the LAMMPS package [40]. Using the values of mass $m$, $\sigma$ and $\epsilon_{\text{hh}}$, we estimate a time scale, $\tau(= \sqrt{\frac{m_{\text{hh}}}{m\sigma^2}}) \sim 0.35$ millisecond. The time step for integration is taken to be $0.001\tau$. The damping term is taken as $\frac{1}{\gamma} = 10\tau$. All the quantities are averaged over five different independent trajectories each 6500$\tau$ long. We take $L_x = 30\sigma$ and $L_y = 20\sigma$, in the $x$- and $y$-directions, respectively, with the periodic boundary conditions (PBC) and no PBC in the $z$-direction.

**Equilibrium results.** We create an interpenetrating polymer network confined by $h$- and $p$-wall at first. The network consists of 27 identical polymeric strands, each having randomly distributed 50 monomers in a number ratio is $h:p$. The packing fraction of total polymeric beads in our model 0.21. It denotes that about 80% is voids in the system. An equilibrium snapshot of the interpenetrating polymer occurs with $h:p = 50:50$ (25 $p$-beads and 25 $h$-beads), $k = 50$, and $z_p = 5.5$. The network structure is characterised by computing the inter-strand correlation function among the beads belonging to different strands, $C(r)$. This is calculated from the number of beads, belonging to two different strands, within a separation $r$ to $r + dr$, normalized by the corresponding shell volume and averaged over configurations. $C(r)$ gives information on how the bead in a given strand is surrounded by beads of the other strands and hence, the peak height in $C(r)$ at $r = 1$ gives an estimate of how the chains are linked among each other. While calculating the distance between two beads, we do not include periodic boundary condition in the confining $z$-direction. The $C(r)$ data in (SM, fig. S2) shows a sharp first peak at $r = 1$ which is the signature of an interpenetrating network.

Then we insert TCPs through grand canonical Monte Carlo (GCMC) at a chemical potential and temperature corresponding to volume fraction (0.47) in bulk liquid phase near the $h$-wall (see SM for details). We study their motion within the network in the absence of external force. We set $\bar{\epsilon} = 3.3$ while keeping the other parameters the same as in the interpenetrating polymer. We calculate the
density profile $\rho_\tau(z)$ of the TCPs, by counting the number of tracer particles along strips of width $\delta z$ parallel to the transverse plane and dividing the number by the volume of the strip. Figure 2(a) shows the tracer density profile $\rho_\tau(z)$. We observe distinct peaks along the $z$-direction, the strongest near $h$-wall. The peak near the $h$-wall denotes particles stopped due to the geometrical effect. We numerically integrate this peak $N_h$ and divide it by total number of TCPs $N_{tot}$. We plot $Q = 100(1 - \frac{N_h}{N_{tot}})$ with $\sigma_\tau$ in fig. 2(a) (inset). This quantity goes to zero if no tracer can permeate into the network. The corresponding TCP diameter estimates the mean pore size of the network. The data shows that $Q$ linearly falls with $\sigma_\tau$. The linear extrapolation of this quantity to zero gives an estimate of the mean pore size of the network ($\approx 2$).

**Permeation of tracer colloidal particles in steady-state condition.** Next we apply a driving force along the $+z$-direction on the TCPs. We restrict ourselves to the range $F_0 = 1$–10 for an experimentally comparable pressure drop ($\approx 1$ Pa to 10 Pa) with about 600 TCPs of 1µm order. Permeability $P(\%)$ through the network is obtained by numerically integrating the density profile under the peak close to $z_p$. We show in fig. 2(b) that change in $P$ with time for $\sigma_\tau = 1.5$ for different $F_0$. All curves saturate at large times, which ensures the steady state. We define the saturation time $t_s$ from fig. 2(b) when $P$ reaches 50% of the saturation value. In fig. 2(c) we show that $t_s$ for $\sigma_\tau = 1.5$ decreases with $F_0$ with a power law dependence with an exponent $-0.36$. $t_s$ increases linearly with $\sigma_\tau$, for $F_0 = 1.0$, as shown in fig. 2(d). Converting to physical units we find that for $\sigma_\tau = 1.5$, $t_s \approx 0.6$ s. This compares well to normal healthy human breathing time.

In order to understand the nature of the permeation process, we explore the temperature dependence of $P$. We consider the saturated value of $P$ for a given condition. The ln $P$ vs. $1/T^*$ plot for $\sigma_\tau = 1.5$ and different $F_0$ in fig. 3(a) shows a linear fall, suggesting an activated Arrhenius process [41]. The slope of the linear dependence gives the activation barrier $F_B$. We show similar data for $\sigma_\tau = 1.2$ for $F_0 = 1.0$ in fig. 3(a). Here the line is almost flat, denoting that the TCPs of this size experience almost no barrier. The barrier $F_B$ is sensitive to $F_0$ as well. We show in fig. 3(b) that $F_B$ varies linearly with $F_0$ for $\sigma_\tau = 1.5$. We find that the barrier height $F_B$ is insignificant for $\sigma_\tau = 1.2$ (data not shown) for all $F_0$.

Next we consider the microscopic origin of $F_B$. We compute the potential energy profile along the $z$-direction per tracer particle, averaged over steady-state configurations. $V_H(z)$ is the potential energy profile for the interaction of the TCPs with the h-beads, $V_P(z)$ that with p-beads and the total potential energy, $V(z) = V_H(z) + V_P(z)$. We show in fig. 3(c) $V_H(z)$, $V_P(z)$ and $V(z)$ vs. $z$ for $\sigma_\tau = 1.2$ with $F_0 = 1.0$ (main panel) and $\sigma_\tau = 1.5$ (inset). We find that both $V_H(z)$ and $V_P(z)$ are almost flat, but $V_P(z)$ is deeper than $V_H(z)$ and $V(z) \approx V_P(z)$. Thus, $V_P(z)$ is primarily responsible for the energy barrier. A larger TCP experiences more p-beads in the course of its motion to experience a deeper energy landscape than smaller TCPs which we observe in fig. 3(d) for $\sigma_\tau = 1.5$ for the same
Fig. 4: (a) $V_P(z)$ vs. $z$ plot with $T^* = 1.0$ for $k = 50$, $z_p = 5.5$, $F_0 = 1.0$ for $\bar{\epsilon} = 3.3$ (black line); $\bar{\epsilon} = 2$ (grey dotted line) and $\bar{\epsilon} = 5$ (black dashed line). (b) $V_P(z)$ vs. $z$ plot with $T^* = 1.0$ for $\bar{\epsilon} = 3.3$, $k = 50$, $z_p = 5.5$ for $F_0 = 1.0$ (black line); $F_0 = 10.0$ (grey line). We divide $\epsilon$ by $F_0$ to ensure the range (0, 1) for both cases.

(3) The localization tendency is opposed by the driving force. The external force helps the TCPs to overcome the $p$-bead interaction energy. We illustrate the energy profile in the presence of external drive in fig. 4(b). We fix $\sigma_{tr} = 1.5$ and $\bar{\epsilon} = 3.3$ and vary $F_0$. A deeper minimum is observed in $V_P(z)$ close to the $p$-wall at a higher $F_0(=10.0)$ compared to a lower $F_0(=1.0)$. This shift helps the TCPs to move closer to the $p$-wall, increasing $P$.

(4) We also plot the energy profile $V_P(z/z_p)$ vs. $z/z_p$ for two different confinement lengths keeping the monomer density the same as in fig. 4(d). We divide $z$ with confinement length $z_p$ to ensure the range (0, 1) for both cases. We observe that for large $z_p(=16.5)$, deeper minima are observed close to the $p$-wall with a relatively flat profile elsewhere compared to lower $z_p(=5.5)$. So, particles easily pass through the network in a less confined system.

Fig. 5: (a) $\sigma_{tr}$ vs. $p$ plots of $\sigma_{tr} = 1.5$ with $T^* = 1.0$, $k = 50$, $z_p = 5.5$, $F_0 = 1$, for $\bar{\epsilon} = 0.5$ (open circles). The black line is a guide to the eyes; $\bar{\epsilon} = 5.0$ (black squares). The dotted line is a guide to the eyes. (b) $C_{max}$ vs. $p$ plots with $T^* = 1.0$, $\epsilon_{wh} = 1.0$, $\epsilon_{pp} = 0.33$, $\epsilon_{wh,wh} = 0.33$, $\epsilon_{pp,pp} = 0.33$, $\epsilon_{wh,pp} = 0.033$, $k = 50$, $z_p = 5.5$. (c) $e$ vs. $k$ plot (solid circles) for $\sigma_{tr} = 1.5$ with $T^* = 1.0$, $kp = 50$; $F_0 = 1$, $\bar{\epsilon} = 3.3$, $z_p = 5.5$. The solid line represents the best fit and the dotted line is a guide to the eyes. Inset: pair correlation function of beads belonging to different two polymeric strands $C(r)$ vs. $r$ for $k = 50$ (dotted black line) and $k = 500$ (grey line). Other parameters are the same as in panel (c).

**Mask efficiency.** – Next we illustrate how the mask efficiency $e$ can be tuned by the network properties. Mask efficiency is defined by $e(\%) = 100 - P(\%)$. The lower the value of $P$, the lower the number of tracer particles penetrating into the region close to the $p$-wall, meaning better efficiency of the FM to intercept the TCPs. We fix the temperature at the room temperature ($T^* = 1.0$), fix the breath-ability condition ($F_0 = 1.0$) and consider the droplet size in the micrometer range ($\sigma_{tr} = 1.5$). We observe changes in $e$ varying $\bar{\epsilon}$ for different composition, namely, the $kp$ ratio. We show the $e$ vs. $p$ plot for both low and large $\bar{\epsilon}$ in fig. 5(a). For low $\bar{\epsilon}(=0.5)$ $e$ decreases linearly with $p$. For larger $\bar{\epsilon}(=5.0)$ $e$ is higher than that with lower $\bar{\epsilon}$ for all $h$. Moreover, $e$ has a maximum for this $\bar{\epsilon}$ at $p = 50\%$.

In order to understand the composition dependence, we note that there are competitive aspects. We show the first peak height of the inter-strand correlation function, $C_{max}$ as a function of $p$ in fig. 5(b) which clearly shows a linear fall of $C_{max}$ with $p$. Note that an increase in $p$ means a decrease in $h$. Since $h$-beads ensure the inter-strand connectivity in the network, the connectivity decreases with increasing $p$. This allows the TCPs to permeate through the network more easily. The fall in $e$ for low $\bar{\epsilon}(=0.5)$ follows this trend particularly for large $p$. On the other hand, larger $\bar{\epsilon}$ creates a larger barrier to the TCP movement as
observed in fig. 4(a). These two opposing tendencies control the composition dependence of \( \varepsilon \). For larger \( \varepsilon = 5.0 \), the competing effects result in the maximum at certain \( p \) value.

We also examine how the rigidity and confinement length \( z_p \) affect \( \varepsilon \). We plot \( \varepsilon \) with \( k \) in fig. 5(c). We observe a linear increase in \( \varepsilon \) with \( k \) and saturation for large \( k \). Unlike the case of fig. 5(b) there is no such significant change in the interpenetration property of the network for different rigidities as shown by \( C(r) \) for different \( k \) values in the inset of fig. 5(c). We further compute the normal (zz) component of the pressure tensor (see details in the SM) of the network beads as a function of \( z \). The normal pressure profile \( P_{zz}(z) \) in fig. 5(d) shows peaks close to both walls. The peak of \( P_{zz}(z) \) close to the p-wall increases with rigidity. Thus, the network resists to more particles from passing through it towards the p-wall with increasing \( k \) resulting in enhanced efficiency. This is consistent with deeper \( V_p(z) \) in fig. 4(c) observed for large \( k \). In other words, a large \( k \) allows a better interaction of the network with the TCP.

In order to examine how the thickness of the network region affects \( \varepsilon \), we increase \( z_p \) keeping the monomer density fixed. We plot \( \varepsilon \) with \( z_p \) in fig. 6(a). We find that as \( z_p \) increases, \( \varepsilon \) decreases linearly and eventually gets saturation beyond \( z_p = 16.5 \). The inset of fig. 6(a) shows that (SM, fig. S3) \( C_{max} \) linearly drops with \( z_p \) up to \( z_p = 16.5 \) after which the bulk limit (see details in SM) sets in. Thus, the system gets less confined, the network structure gets loose. A loose network provides a flat \( V_p(z) \), as shown in fig. 4(d), and better mobilities of the TCPs and hence, poorer \( \varepsilon \).

Our results suggest that large efficiency can be achieved by a deeper \( V_p(z) \) profile. For instance, 95% efficiency in intercepting tracer micro-droplets under normal breath-ability condition at room temperature can be achieved as follows: 1) Composition of \( h:p = 50:50 \), keeping the network structure sufficiently robust. 2) \( \varepsilon > 3 \) to allow large interaction of the p-beads with the TCPs. 3) Fairly rigid network (\( k \geq 200 \)); and 4) \( z_p \sim \) few microns so that the network remains sufficiently strong to resist the TCP penetration. The void space in the network should be sufficient to allow movement of small molecules \( \sigma_{tr} < 1.2 \). So far we have calculated tracer permeation during inhalation cycle. Now we consider exhalation with FM on. Using parameters for \( e \sim 95\% (\varepsilon = 3.3, F_0 = 1.0, T^* = 1.0, k = 200, \) and \( z_p = 5.5 \)) we put TCPs with \( \sigma_{tr} = 1.5 \) close to the p-wall as done previously. We apply driving force from p-wall to h-wall. We find in fig. 6(b) that the \( P \) at the h-wall increases linearly with \( F_0 \). Thus, TCPs are efficiently drained away.

Conclusions. – To summarize, we study the permeation of TCPs within a network of polymers in the presence of a driving force, using Langevin dynamics simulations. The parameters in our studies are chosen so as to ensure breath-ability conditions in a FM. We find that the droplet permeation through the network is an activated process. The activation barrier increases with 1) increasing tracer size, 2) decreasing driving force and 3) increasing network-tracer interactions. The barrier height is mainly determined by the magnitude of the more favourable interaction experienced by the TCP in the network. For a given tracer size, driving force and temperature, the efficiency of the mask depends on: 1) \( h:p \) ratio, 2) increasing interaction strength of tracer and p-beads, 3) increasing the rigidity and 4) decreasing the thickness of the network. Our model is sufficiently robust to be helpful in designing a mask with better efficiency while retaining normal breath-ability conditions. We do not include the electrostatic interaction in our model. However, it may be interesting to take a charge bead of a FM network to observe long-range the electrostatic effect in the efficiency of a FM in the future. It may be also worth taking into account the shape of the size change of micro-droplets to observe more realistic transport inside a FM in future.

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Data availability statement: The data that support the findings of this study are available upon reasonable request from the authors.

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Model studies on motion of respiratory droplets driven through a face mask

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