Extended friction elucidates the breakdown of fast water transport in graphene oxide membranes

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Abstract – The understanding of water transport in graphene oxide (GO) membranes stands out as a major theoretical problem in graphene research. Notwithstanding the intense efforts devoted to the subject in the recent years, a consolidated picture of water transport in GO membranes is yet to emerge. By performing mesoscale simulations of water transport in ultrathin GO membranes, we show that even small amounts of oxygen functionalities can lead to a dramatic drop of the GO permeability, in line with experimental findings. The coexistence of bulk viscous dissipation and spatially extended molecular friction results in a major decrease of both slip and bulk flow, thereby suppressing the fast water transport regime observed in pristine graphene nanochannels. Inspection of the flow structure reveals an inverted curvature in the near-wall region, which connects smoothly with a parabolic profile in the bulk region. Such inverted curvature is a distinctive signature of the coexistence between single-particle zero-temperature (noiseless) Langevin friction and collective hydrodynamics. The present mesoscopic model with spatially extended friction may offer a computationally efficient tool for future simulations of water transport in nanomaterials.

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Introduction. – Water transport through graphene-derived membranes has recently captured much attention due to its promising potential for many technological applications, such as water filtration, separation processes, and heterogeneous catalysis and chemical sensing [1–4]. A number of simulations have shown that fast water permeation through carbon materials, such as carbon nanotubes (CNT [5,6]) and pristine graphene membranes [7], is due to the slip flow at the water-carbon interface. Fast water transport (FWT) with permeabilities higher than 10 Lm−2h−1bar−1 [8–10] has also been reported for graphene oxide laminate (GOL).

However, in contrast to pristine graphene and CNT, a clear consensus on the GO fast water transport mechanism has yet to emerge [7,11–13]. To date, departures from hydrodynamic (i.e., Hagen-Poiseuille) behavior are typically attributed to the low friction experienced by water in atomistically smooth graphene nanochannels [14] or to the presence of structural defects in GOL, leading to shorter water paths [15]. The latter hypothesis is further corroborated by the breakdown of FWT from molecular interactions of water with basal plane hydroxide and epoxide groups, which hinders the motion of water molecules. This phenomenon was recently reported in non-equilibrium molecular-dynamics simulations of flows inside graphene oxide (GO) nanochannels [15,16]. Under such conditions, slip-corrected continuum hydrodynamics is expected to provide a correct description of the aforementioned transport mechanism. However, at the hydrodynamic level the details of the slip corrections must be imposed a priori because the physics of slip flow is governed by non-equilibrium phenomena. Such details can certainly be accounted for by a fully atomistic approach, but at the price of prohibitive computational costs. All of the above lead to an ideal scenario for mesoscale modeling techniques, which may offer a valuable
compromise between physical fidelity and computational viability [17–19].

In this work, we explore water permeation in GOL via mesoscale simulations. Furthermore, we provide a direct calculation of the membrane’s permeability, which is drastically lower than the one observed in pristine graphene characterized by FWT. Our simulations exhibit satisfactory agreement with experimental GOL permeability and also provide values of the slip length on par with recent non-equilibrium molecular-dynamics simulations (NEMD) [16]. More precisely, we demonstrate that a suitably simplified (lattice) kinetic model proves capable of predicting the breakdown of FWT, namely the macroscopic permeability of the GO membrane, as well as the slip phenomena, at a very affordable computational cost. For instance, a baseline simulation takes only a few CPU hours on a high-end PC.

Method. — GO was synthesized by modified Hummers’ method [20] and dispersed in ethanol at a concentration of 0.1 mg/L. Additional details can be found in the supporting information Supplementarymaterial.pdf (SI). The solution was then bath sonicated for 5 minute in a Branson 2510 Ultrasonic cleaner. 1 ml of the sonicated GO solution was deposited on a porous polyvinylidene difluoride (PVDF) membrane (pore size = 200 nm) via vacuum filtration. The membranes were then characterized by using a Zeiss ULTRA Field Emission Scanning Electron Microscope (SEM) with an In-lens detector (see figs. S 1 and S 2 in the SI). Scanning electron microscopy and mass analysis suggest the formation of a circa 30 nm thick GO layer on top of the PVDF membrane. The crystallographic structure of the membranes was analyzed with a Bruker D8 equipped with a two-dimensional VANTEC-500 detector. The spectra were obtained by the integration of the 2D diffraction pattern image (see fig. S 3 in the SI) via EVA software. Depending on the sample, the integration time was between 600 and 1200 seconds. Permeability results were carried out with a custom-made dead-end filtration system operating at a maximum pressure of 3.5 bar. In particular, a 2 cm in diameter GO membrane was cut and placed in a stainless-steel EDM Millipore filter holder. The pressure was monitored with an Ingersoll pressure gauge regulator (see fig. S 4 in the SI). The numerical simulations are based on the lattice Boltzmann (LB) method, augmented with a novel zero-temperature (noiseless) Langevin frictional force accounting for the GO-water interactions. Since the LB method is largely documented in the literature [21–23], in the following we discuss only its basic features. The lattice Boltzmann equation reads as follows:

\[
f_i(\vec{x} + \vec{c}_i \Delta t, t + \Delta t) = (1 - 1/\tau) f_i + 1/\tau f_i^c + \Delta f_i, \tag{1}
\]

where \( f_i(\vec{x}, t) \) is a set of discrete probability distribution functions (PDFs) representing the probability of finding a molecule at position \( \vec{x} \) and time \( t \) with a lattice-constrained velocity \( \vec{c}_i \), where the index \( i \) runs over the nine directions of the lattice [24]. \( f_i^c \) is the set of discrete local Maxwellian equilibria (i.e., truncated low-Mach-number expansion of the Maxwell-Boltzmann distribution) [21] and \( c_s \) is the speed of sound of the model [24]. In the above equation, the left-hand side is the lattice transcription of molecular free flight along the lattice directions, while the right-hand side describes collisional relaxation towards local equilibrium, described by a low-Mach-number expansion of the Maxwell-Boltzmann distribution. The relaxation parameter \( \tau \) controls the kinematic viscosity of the lattice fluid through the relation \( \nu = c_s^2 (\tau - 1/2) \) in lattice units \( \Delta x = \Delta t = 1 \). The last term, \( \Delta f_i \), is the correction due to the friction exerted by the hydroxyl and epoxi (see fig. 1(b)) on the the GO flake’s length, \( 2h \) is the spacing between two GO layers and \( w \) is the spatial extent of the frictional force. The red area in the GOL structure identifies the elementary periodic cell used in the simulation. As shown in panel (b), hydroxide and epoxide groups interact with the water molecules slowing down their motion inside the GO nanochannel (panel (a)). In the sketch, \( L \) is the GO flake’s length, 2\( h \) is the spacing between two GO layers and \( w \) is the spatial extent of the frictional force. The vertical motion is hindered by a series of horizontal staggered plates (GO flakes), which force the water molecules to follow a tortuous path from inlet to outlet ports.
water molecules and can be expressed as $\Delta f_i = w_i \frac{F_i}{\sqrt{t}}$, in which $w_i$ is the set of weights for the chosen lattice [21], and the frictional force is taken in the following form [25]:

$$F = -\rho \gamma(y) \vec{u},$$

(2)

where $\rho$ and $\vec{u}$ are the fluid density and velocity, respectively, and the heterogeneous friction coefficient reads as follows:

$$\gamma(y) = \gamma_0 (e^{-\frac{y}{\delta}} H_L(y, \delta) + e^{\frac{y-h}{\delta}} H_R(y, \delta)),

(3)

where $w$ is a representative size of the protruding functional groups and $\gamma_0$ is a characteristic water-hydroxyl collision frequency, taken equal to 0.2 (in lattice units) in all the simulations. The value $\gamma_0 = 0.2$ in LB units corresponds to a friction time scale $\tau \sim 1.5 \times 10^{-14}$ s, which is comparable with the collisional time scale of water molecules, $\tau_W \sim 70$ ps$^{-1}$. This comes from the conversion between LB and physical units, namely $\gamma_{phys} = \gamma_{LB}/dt$, where $dt = 3 \times 10^{-15}$ s. These values can be found in the literature (see [26,27]). Thus, the value of $\gamma_0$ has been chosen so as to match the characteristic water-water collision frequency value, which can be determined via MD simulations by monitoring the velocity auto-correlation function [26].

The wall function $H_L(y)$ takes the value 1 for $0 < y < \delta$ and 0 elsewhere. Likewise, $H_R(y) = 1$ for $2h - \delta < y < 2h$ and 0 elsewhere. The reference case is $\delta = w$ (truncated Langevin throughout the text). In this case, if $w < h$, the frictional force drops discontinuously to zero in the central region of the channel, $w < y < 2h - w$. To regularise this discontinuity, we also consider the case $\delta = h$ (non-truncated Langevin). The physical idea behind the noiseless Langevin frictional force is to account for the complex water-GO molecular interactions at a coarse-grained level, whereby all atomistic details are channelled into the parameters $\gamma_0$ and $w$.

Whether the contact angle and the slip length can be treated as independent variables still is an open question in the current literature (see [28,29]). In line with the mesoscale nature of our model, we assume sufficient universality to support a direct correlation between the water-graphene contact angle and the slip length. This said, from the NEMD results (fig. 4d in [11]), we read off a slip length between 0.3 and 1.0 nm with a 40% to 5% of graphene contact angle and the slip length. This said, the extension to support a direct correlation between the water-graphene and the heterogeneous friction coefficient reads as follows:

$$\Delta x = 10^{-10} m,$

yielding a time step $\Delta t \sim 3 \times 10^{-15}$ s. Note that sub-molecular spatial resolutions are typical of LB simulations of nanoflows [30]. The time step, however, is about an order of magnitude larger then the time steps typically used in MD simulations of flows through GO interlayers [11]. It is also worth mentioning that the CPU time needed to update a single molecule is significantly larger than the one required to advance a single LB cell, because the cell contains less neighbors and, more importantly, such neighbors are fixed in space, hence there is no need to recompute the interaction list at every time step [31]. Moreover, LB requires no statistical averaging, since it is based on a pre-averaged probability distribution function. In addition, LB is often more efficient than computational fluid dynamics because i) pressure is available locally in space and time, with no need of solving a demanding Poisson problem, ii) transport is exact, since free streaming proceeds along fixed molecular velocities instead of space-time-dependent material streamlines, iii) diffusion is emergent, hence it does not require second-order spatial derivatives, thus facilitating their formulation of boundary conditions in confined flows [23].

Results. – Assuming the GOL structure to be symmetric and periodic [7,10] (see red area in fig. 1(a)), we consider only two nanochannels out of the full device. A similar geometry set-up has been recently employed to investigate water permeation through graphene-based membranes by means of MD simulations [32]. These two channels are connected via two openings of half the width of the inlet/outlet pores (see fig. 1(a)). The boundary conditions at the left-right and top-bottom surfaces are periodic, to simulate the proximity of two adjacent GO layers. At solid walls, the molecules experience the
friction force previously described. We have run several simulations with different values of \( w \). The grid resolution is \( 10000 \times 20 \), corresponding to a flake length of \( 10^{-6} \) m, which we take as a representative experimental value [33]. The mesoscale model was tested against experimental measurements of permeability. The permeability of the membrane is defined as \( \kappa = \mu u_s / |\nabla p| \), where \( \mu \) is the dynamic viscosity, \( \nabla p \) the pressure gradient across the membrane and \( u_s \) the superficial velocity defined as the ratio between the membrane discharge per unit area. It is worth recalling that in the Darcy regime, the permeability \( \kappa \) is pressure independent (see fig. S 5 in the SI). In order to test our numerical results against experimental data, we inferred the experimental values of flow rates (mass flow per unit time) from the permeate vs. time plot, reported in fig. 2, for different values of the applied pressure. From these data, we compute a dimensionless permeability \( \kappa^* = \kappa / (2h)^2 \), where \( 2h \) represents the spacing between two GO layers. X-ray diffraction measurements give \( 2h \approx 0.8 \) nm. The experimental value of the dimensionless permeability \( \kappa^* \) for a \( \approx 30 \) nm thick membrane of diameter \( d = 2 \) cm is \( \kappa^* \approx 2.8 \times 10^{-4} \), corresponding to a permeability of \( 3.6 \pm 0.5 \) LMH/bar. This value of permeability is in line with data previously reported for ultrathin (<50 nm) GO membranes (see [8,20]) and represents a promising result for nanofiltration applications. It is important to underline that higher values of permeability, as high as \( 20 \) LMH/bar (\( \sim 4 \) times higher than those obtained in our experiments), have been achieved for GO membranes [10]. However, these values can be connected to the presence of defects or larger GO nanochannels due to the chemical modification of the GO membranes [10,34,35]. Higher permeability can also be achieved by intercalating the GO membranes with high-aspect-ratio nanoarchitectures, such as CNT [11,36].

Figure 3 illustrates two comparisons, for both the truncated and non-truncated Langevin frictions: i) between the permeability obtained by mesoscopic simulations and experiments; ii) between the slip length obtained by NEMD [15] and by this study. The experimental data reported in fig. 3 should not be regarded as being obtained by tuning the characteristic hydroxyl size. Instead, in our simulations, we investigate the behaviour of the extended friction by varying the parameter \( w \), standing for the representative size of the protruding functional group OH. Thus, after the characteristic water-hydroxil collision rate has been fixed (according to values reported in the literature, [26]), the only free parameter to be set is \( w \). The case \( w = 0 \) corresponds to a simulation without the noiseless Langevin friction, \( i.e., \) pure “free-slip” hydrodynamics. By “free-slip” we mean boundary conditions which leave the flow momentum tangential to the wall unchanged. This is representative of the FWT regime observed in pristine graphene experiments. Note that the flow still reaches a steady-state solution on account of the localized dissipation experienced at the sharp 90° turns between two subsequent layers, visible in fig. 1(c). The main outcome from fig. 3 is a dramatic drop in permeability of two orders of magnitude, already at \( w = 0.1 \) nm, \( i.e., \) \( w/h = 0.25 \). Such a dramatic drop in permeability is consistent with experimental observations that report a suppression of FWT regimes in the presence of hydroxyl groups. Further increments of \( w \) lead to a sizeable reduction in permeability by ca. one order of magnitude, from \( w = 0.1 \) nm to \( w = 0.4 \) nm. It is worth noting that the employed resolution (\( \Delta x = 0.1 \) nm) poses a constraint on the lower bound of \( w \). We note that the truncated \( (\kappa_w, \delta = w) \) and non-truncated \( (\kappa_h, \delta = h) \) scenarios yield nearly the same picture with only minor quantitative variations. Moreover, fig. 3 shows that for both the truncated and non-truncated scenario, the slip length remains between 0.5 nm and 2 nm, in agreement with the values provided by NEMD [15]. It is worth noting that the best match of the experimental (permeability) and NEMD (slip lengths) results with the simulations is obtained when \( w \) is between 0.1 nm and 0.2 nm (\( i.e., \) \( w/h = 0.25-0.5 \)), which agrees with the physical dimension of the oxygen functionalities in the GO nanochannels [37]. This further corroborates
the validity of the model and its potential to capture the physical phenomena in 2D nanostructured inspired materials within an efficient computational framework.

**Inside the flow structure.** Next, we proceed to inspect the internal structure of the flow. In particular, we focus on the occurrence of slip flow in the presence of hydroxyl, as recently observed in non-equilibrium molecular-dynamics simulations [15]. As previously discussed, slip flow is a typical manifestation of individual non-hydrodynamic behavior driven by non-equilibrium effects near the wall. To glean quantitative insights into such non-equilibrium phenomena is informative for inspecting the one-dimensional cross-flow profiles \( u_x(y) \) for different values of \( w \) vs. the case of free-slip boundary conditions. Figure 4(a) illustrates that the flow profiles display a Poiseuille-like parabolic trend in the bulk region, smoothly turning into a flat profile near the wall, with a positive curvature and a small non-zero slip velocity. The comparison between the pristine graphene profile with the other profiles highlights the major drop of mass flow due to the noiseless Langevin friction. The increase of \( w \) leads to the suppression and flattening of the water profiles. From the velocity profiles, we compute the slip length according to \( L_s = \lim_{y \to 0} \left| \frac{u_x(y)}{\nabla_y u_x(y)} \right| \). As previously discussed for fig. 3, we confirm the presence of a residual slip length, which is small in absolute physical units, but fairly sizable in units of the channel width \( h \), namely \( L_s/2h \sim 0.5 \). Furthermore, the effect of the different cut-off lengths employed in the truncated (\( \delta = w \)) and non-truncated (\( \delta = h \)) Langevin is minor, leading to slight differences in both the membrane permeability and slip lengths. To further test the robustness of this approach in fig. 4(b) we report a comparison between the velocity profiles obtained by the noiseless Langevin-LB and the MD approach [11] for a 3 nm wide GO channel, showing an outstanding agreement between the two models.

We conclude this letter with an ex-post analysis of our mesoscale model in the light of the numerical results discussed above. First, we note that both friction and viscous dissipation withstand the driving action of the pressure gradient, they operate according to very different and competing mechanisms. Friction drives the fluid towards the following local flow configuration:

\[
    u_x^{(L)}(y) = \frac{\nabla_x p}{\rho \gamma(y)}. \tag{4}
\]

This results in a slip flow \( u_{\text{slip}} = |\nabla_x p| / (\rho \gamma_0) \) (independent of \( w \)) at the wall and the corresponding slip length is \( L_s = w \). Viscous dissipation, on the other hand, drives the fluid towards a parabolic Hagen-Poiseuille profile,

\[
    u_x^{(H)}(y) = u_H \left[ \frac{y}{h} \left( 2 - \frac{y}{h} \right) + \text{const} \right], \tag{5}
\]

where we have set \( u_H = \frac{\nabla_x p}{\rho \gamma H} \). The above hydrodynamic solution is compatible with either slip or no-slip flow conditions, depending on the value of the constant on the right-hand side. In slip hydrodynamics \( \text{const} = L_s/h \), so that \( L_s/h \to 0 \) recovers standard no-slip hydrodynamics. This value can only be prescribed a priori, exposing the weakness of the hydrodynamic approach previously mentioned.

The two profiles, \( u_x^{(L)}(y) \) and \( u_x^{(H)}(y) \) cannot coexist in nothing but an intermediate compromising form, resulting from the smoothing of the noiseless Langevin profile due to viscous dissipation. To gain a deeper understanding, in fig. 5 we report the friction and viscous forces separately, for the case \( w = \delta = 0.2 \) nm. As one can see, the bulk...
flow is dominated by viscous dissipation (friction is zero in the bulk because $\delta = 0.2 \text{nm}$), while in the vicinity of the positive curvature of the flow profile, friction takes over. However, the two contributions become comparable but opposite in sign due to the exponential decay of the extended friction, thus exhibiting the observed inverted (positive) curvature. Because of the exponential decay of the extended friction, the near-wall region is still dominated by viscous dissipation, as reflected by the bulk parabolic profile clearly visible in fig. 5. The onset of the inverted curvature is a distinctive signature of the coexistence between single-particle noiseless Langevin friction and collective hydrodynamics. This extra-freedom is key to recover the inverted curvature profile.

**Conclusions.** – In summary, our numerical simulations portray the following picture. Even a small amount of spatially extended noiseless Langevin friction, $w/h = 0.25$, leads to a dramatic drop in the mass flow compared to free-slip hydrodynamics. Such friction still supports a small residual slip flow at the wall, with a slip length of the order of the friction length $w$. However, this flow is largely negligible compared to the free-slip in the absence of friction. The net result is a dramatic loss of permeability due to the presence of the functional groups, hence the inhibition of the FWT regime observed in pristine graphene membranes. Viscous effects dominate the bulk flow and contribute to the smoothing of the sharp features of the flow due to the presence of the hydroxyl and epoxy. Inspection of the flow structure reveals an inverted curvature in the near-wall region, which connects smoothly with a parabolic profile in the bulk region. Such inverted curvature is a distinctive signature of the coexistence between single-particle noiseless Langevin friction and collective hydrodynamics.

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