Atomic Scale Interfacial Transport at an Extended Evaporating Meniscus

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Supporting Information

ABSTRACT: Recent developments in fabrication techniques have enabled the production of nano- and Ångström-scale conduits. While scientists are able to conduct experimental studies to demonstrate extreme evaporation rates from these capillaries, theoretical modeling of evaporation from a few nanometers or sub-nanometer meniscus interfaces, where the adsorbed film, the transition film, and the intrinsic region are intertwined, is absent in the literature. Using the computational setup constructed, we first identified the detailed profile of a nanoscale evaporating interface and then discovered the existence of lateral momentum transport within and associated net evaporation from adsorbed liquid layers, which are long believed to be at the equilibrium established between equal rates of evaporation and condensation. Contribution of evaporation from the adsorbed layer increases the effective evaporation area, reducing the excessively estimated evaporation flux values. This work takes the first step toward a comprehensive understanding of atomic/molecular scale interfacial transport at extended evaporating menisci. The modeling strategy used in this study opens an opportunity for computational experimentation of steady-state evaporation and condensation at liquid−vapor interfaces located in capillary nanoconduits.

■ INTRODUCTION

Capillary evaporation and the associated passive liquid flow are vital for numerous natural and artificial processes such as transpiration of water in plants,1 solar steam generation,2,3 water desalination,4,5 microfluidic pumping,6 and cooling of electronic and photonic devices.7 Regardless of the process or the geometrical configuration, studies on evaporation focus on identification and characterization of heat transfer and flow dynamics in the vicinity of the contact line, the juncture of three phases of matter. Figure 1a−c shows different evaporation processes schematically. Green dashed rectangles point out the liquid film distribution around the contact line, which is broadly composed of three multiscale regions as shown in Figure 1d. The evaporation rate intensifies in the evaporating thin-film region because of the microscale liquid film thickness. The adsorbed nanoscale layer extending further is assumed to be nonevaporating because of the suppression of evaporation by strong long-range intermolecular forces.8−20 While the kinetic theory of gases21,22 has been widely used to predict the theoretical maximum rate of evaporation, experiments have always calculated smaller heat fluxes than the kinetic limit.23 However, two recent experimental studies have attracted the attention of scientific community by reporting evaporation fluxes 1−2 orders of magnitude higher than the prediction of kinetic theory.24,25 These unexpectedly high flux values were attributed to the possible underestimation of evaporation area in the first study,24 where the stretching of the water meniscus over the flat surface adjacent to the channel mouth was speculated. On the other hand, the second study25 reported evaporation rates from a water meniscus located at a channel entrance defined by four sharp edges, which eliminate the possibility of outstretching of the meniscus. Moreover, extension of the meniscus within the channel was also
The evaporative mass loss, whereas the interface at the cooling zone is expanded because of the condensing heating and cooling zones, respectively. The length of these parts is equal to the channel height. The interface at the heating zone is carved because of the reduced liquid film resistance. Changes in the capillary and disjoining pressures govern the liquid flow in this region. Film thickness is at the nanoscale within the adsorbed layer.

Estimated by using a model in the literature, and the evaporation area was modified accordingly. Regardless of the increased evaporation area, estimated heat fluxes still exceeded the kinetic theory limit, indicating the need for fully understanding the characteristics of an evaporating contact line. Undoubtedly, an accurate calculation of the evaporation flux depends on the precise estimation of the effective surface area of evaporation, which is extremely challenging to quantify because of lack of information about the molecular/atomic nature of the evaporating contact line. Thermal scientists have long believed that the adsorbed tail of the evaporating contact line does not possess a net evaporation rate. While theoretical studies assumed a balance between evaporation and condensation rates and calculated the equilibrium adsorbed film thickness based on the minimum free energy principle, a considerable amount of experimental effort has been devoted to observe the vicinity of the contact line. Most recently, Mehrizi and Wang detected extremely stretched nanofilms of thickness 2–6 nm attached to a water droplet evaporating to its own vapor and 0–10 nm thick films attached to a formamide droplet evaporating in air. Morphological distinction between the intrinsic meniscus and nanofilms was apparent in all of their experiments. Therefore, they defined the contact line as the intersection of the intrinsic meniscus and the nanofilm. Within the water nanofilm, they detected a thinning transition film close to the contact line and a near constant thickness adsorbed film attached to the end of the transition film. They characterized the transition film as evaporating because of its thickness variation and the adsorbed region as nonevaporating because of its near flat profile. Due to the observation of long nanofilms beyond the contact line, we consider this experimental work as a clue suggesting a possible area enlargement for the evaporation. However, identification of the effective evaporation area, especially in a few nanometers or sub-nanometer interfaces where the adsorbed film, the transition film, and the intrinsic region are intertwined, is impractical for optical and electron microscopies because of their nanoscale resolution and operating conditions. Therefore, a comprehensive description of the evaporation mechanism on this scale is missing.

Figure 1. Schematics of (a) an evaporating droplet, (b) evaporation from a capillary, and (c) bubble growth. Green dashed rectangles point out the region near the contact line, where the evaporation rate intensifies because of the decreased liquid film thickness. (d) Liquid forms three multiscale regions around the contact line. Film thickness is at the macroscale within the intrinsic meniscus region. Capillary pressure gradient, arising from the curvature changes, drives the flow in this bulk region. Film thickness is at the microscale within the evaporating thin-film region, where the evaporation rate intensifies because of the reduced film resistance. Changes in the capillary and disjoining pressures govern the liquid flow in this region. Film thickness is at the nanoscale within the adsorbed layer.

Figure 2. Computational setup. (a) A snapshot of the isothermal configuration. Liquid phase of the saturated argon mixture (blue spheres) confined between solid platinum walls (gray spheres). Distance between the channel walls, D, is 3.92 nm and the length of the channel wall and simulation domain is proportional as shown in the figure. Depth of the simulation domain is 3.72 nm. The walls consist of four atom layers and have a thickness of t = 0.59 nm. (b) Density distribution of the isothermal configuration. Two symmetric and statistically stable liquid–vapor interfaces form at the channel inlets. (c) A snapshot during the equal energy injection/extraction process. Red and blue parts of the wall show the heating and cooling zones, respectively. The length of these parts is equal to the channel height. The interface at the heating zone is carved because of the evaporative mass loss, whereas the interface at the cooling zone is expanded because of the condensing fluid atoms. (d) Density distribution during the equal energy injection/extraction. Both interfaces are statistically stable. The evaporating interface is detached from the channel inlet and receded into the channel. The condensing interface is pushed away from the channel inlet and is nearly flat. Density profiles in (b,d) were obtained after time averaging of MD results.
Figure 3. Liquid–vapor interface profiles for the (a) first and (d) second (fluid-wall interaction energy 10 times increased) simulations. Constant energy is being injected in the red colored walls. Blue lines show the interface. Menisci receded into the channel and are located within (a) and beyond (d) the heating zone. Symmetric adsorbed layers are attached to the menisci at the channel walls. Close-up view of the adsorbed layers for the first (b) and second (e) simulations. A snapshot of atoms that are superpositioned on the time-averaged profile of the adsorbed layers, which consist of (b) a monolayer of fluid atoms for the first and (e) a bilayer of fluid atoms for the second simulation because of the increased fluid-wall binding energy. Surface coordinate, “s,” follows the interface of the adsorbed layer. Regions I, II, and III show the adsorbed layer segments located on the inner channel wall, corner, and side wall, respectively. Mass flow rates along the adsorbed layer for the (c) first and (f) second simulations. Mass flow rate decreases along the adsorbed layer and vanishes at the stagnation plane located at the end of region III (see Figure 5). In the insets, the data points show the variation of the evaporation flux (per unit depth) along the adsorbed layers. Data is presented after applying moving average with 20-data points window size. Uncertainty analysis for the flow rate calculation is provided in Section C of the Supporting Information.

■ METHODS

To grasp the physical mechanism of evaporation in capillary nanoconduits, we used molecular dynamics (MD), which is a common tool to study the physical movement of atoms and molecules. Although MD simulations are suitable for nanoscale physical and temporal dimensions, MD results can be successfully used to predict experimentally determined macroscale system properties.30

A saturated liquid–vapor mixture has equal evaporation and condensation rates at the interface. To disturb the equilibrium, a pressure difference between the bulk vapor and the vapor just above the interface must be generated. In an enclosed system, evaporation can be favored by either reducing the bulk vapor pressure or by increasing the interface pressure. The first method can be applied by continuously removing the vapor phase from the system. If the mixture is composed of water and air, controlling of relative humidity is an example of this procedure as performed by the recent experiments.24,25 However, application of this methodology is not practical for the current investigation. Because of the computational cost of MD simulations, only a limited number of atoms/molecules can be simulated within restricted time spans. Continuous removal of atoms/molecules would decrease the total number of fluid atoms during a simulation. Before the establishment of a steady evaporation, fluid atoms can be totally consumed or can drop below a certain amount, for which statistical averaging will not yield trustable results. Therefore, instead of a transient process, a steady-state process, which preserves the total number atoms/molecules, is more reliable. To realize this, we use the recently proposed phase change-induced pumping mechanism.31 At the evaporator part of this pump, a stable evaporating liquid–vapor interface forms. Continuous heating at this part increases the temperature at the interface. Consequently, evaporation is sustained by the increase of the interface pressure instead of removing the vapor atoms/molecules. Selection of fluid type is also critical. The number of vapor atoms in the gas phase should be large enough for accurate statistical averaging. Therefore, the selected liquid should have a high vapor pressure. Water, for instance, is not a good choice for MD simulations because of its relatively low volatility. Saturated water mixture in equilibrium at room temperature has the ratio of 1/50 000 vapor to total water molecules, which is unfavorable for MD simulations conducted in nanoscale volumes. Our modeling strategy aims to construct steady-state evaporation of a high volatile liquid to realize a statistically reliable evaporation analysis. Therefore, argon was used in our computational experiments because of its high volatility and its suitability to be modelled by Lennard-Jones potential with well-defined atomic interactions.32 As a solid substrate material, we used platinum because of its empirically defined interaction parameters33 and its argonophilic characteristics.

In simulations, first, two symmetric isothermal meniscus structures are created within two parallel platinum walls by condensation of the saturated argon mixture to the liquid phase because of the interaction between fluid and solid wall atoms, whereas the vapor phase of argon occupies the rest of the simulation domain (Figure 2a,b). Then, an equal energy injection/extraction process is applied to solid atoms in the heating/cooling zones located at the opposite ends of the nanochannel (Figure 2c,d). This approach preserves the thermodynamic state of the mixture by ensuring zero net heat transfer to the system. At the end of 40 ns of simultaneous heating/cooling, an extended meniscus and a flat liquid film (both statistically stationary) evolve at the heating and cooling zones of the nanochannel, respectively (Figure 2d). The passive liquid flow through the channel is also steady. Density layering, which is a link to the real world behavior of the system,34,35 is prominent near the walls because of the wall-force-field effect. Further details of MD simulations are provided in Section A of the Supporting Information.

To determine the liquid–vapor interface, the simulation domain is divided into rectangular bins, and the average fluid density is calculated at each bin. Starting from the outer gas-phase region, density of each bin is checked in longitudinal directions, and the first bins, where the bin density exceeds the cutoff density, are marked as the liquid–vapor interface. Cutoff density is selected slightly higher than the density of the first minimum density peak in the liquid phase, which is approximately 22% of the average bulk liquid density within the channel. Selection of a higher cutoff density implies the existence of a nonphysical vapor region within the bulk liquid, which prevents the detection of a continuous liquid–vapor interface. However, selection of a lower cutoff density results in a larger liquid volume and thicker adsorbed layers, which does not affect the proper prediction of the mobility of adsorbed layers. Moreover, it is worth mentioning that calculation of the evaporation rate is independent of the interface selection in our computational setup because of the steady evaporation and the associated steady passive liquid flow within the channel. Rate of evaporation is estimated by calculating the mass flow rate from the liquid state at the midchannel in each simulation.
RESULTS AND DISCUSSION

Location and morphology of the evaporating meniscus are functions of the heating rate. While slight heating yields a negligible meniscus deformation, excessive heating results in the burnout of the heated wall. During simulations, we applied different heating rates to observe the response of the evaporating meniscus. The location and profile of the evaporating meniscus corresponding to different heating loads are determined and qualitatively compared with the results of a recent modeling study\(^{36}\) in Figure S2 of the Supporting Information. The profile shown in Figure 3a evolves under the highest heating rate just before the burnout of the wall. At this heating rate, the liquid meniscus is detached from the channel tips and receded into the channel. However, a thin monolayer still covers the surface of the channel at both inside and side walls. We consider this monolayer as the absorbed layer because of its near flat thickness along the inner wall (4.116 ± 0.392 Å) and side wall (2.744 ± 0.196 Å) surfaces. A close-up view of the adsorbed layer is shown in Figure 3b. To investigate the possible momentum transport within the absorbed layer, mass flow is calculated along the surface coordinate, \(\vec{r}\) (see Section B of the Supporting Information). Strikingly, an atomic level mass flow is apparent within the absorbed layer, as shown in Figure 3c, because of the solid–liquid surface tension gradient originating from the temperature gradient together with evaporation along the evaporator surface.\(^{37}\) The mass flow decreases continuously along the layer and vanishes at the end of the side wall, where actually two opposite molecular streams merge because of the periodic boundary condition. The inset shows the variation of the evaporation flux (per unit depth), which becomes maximum at the corner (region II). Additionally, flow and temperature fields near the evaporating interface are reported in Section D of the Supporting Information.

It should be noted that the pumping mechanism used in the simulations requires proper wetting of the wall to keep the liquid phase within the channel, otherwise the condensed liquid slides over the walls and leaves the channel, which prevents the investigation of argon-phobic systems. However, the effect of elevated argon-phlicity can be easily examined by increasing the interaction strength between the fluid and solid atoms. Figure 3d shows the profile of the evaporating meniscus in the second simulation, where the fluid-wall binding energy is increased 10 times. Because of the increased interaction, the thickness of the absorbed layer is almost doubled (inner wall: 7.840 ± 0.392 Å, side wall: 6.272 ± 0.196 Å) enabling the formation of a second atomic layer on the first one (Figure 3e). Surprisingly, the highest attainable heating rate before burnout is nearly doubled, and the amount of evaporation from the adsorbed layer remains almost constant at \(\sim 170\) atoms per second (Figure 3f), despite the increased attraction between the fluid and wall atoms, which is supposed to prevent evaporation. This interesting observation, indeed, is related to the mobility of the adsorbed layer even at elevated attractive forces (see video, Supporting Information). Although the first atomic layer (closest to the wall) has low mobility under the effect of the wall-force-field, the second layer is subjected to lesser attraction of solid atoms because of the increased distance from the wall and has high mobility similar to the monolayer formed on the wall in the previous simulation. Average evaporation flux (see the inset in Figure 3f) is lower than the one in the first simulation because the adsorbed layer is longer, whereas the total evaporation rate from the adsorbed layer is almost the same (\(\sim 170\) s\(^{-1}\)).

Our simulations have demonstrated that a considerable amount of evaporation can occur at the adsorbed layer (47 and 64% of total evaporating mass for our first and second simulations, respectively), and the effective evaporation area can be much larger than the liquid meniscus area because of the evaporation from adsorbed layers. To quantify the effect of evaporation area selection on the evaporation flux estimations, we calculate the evaporating mass flux for the first simulation using three different evaporation areas, as shown in Figure 4.

The simplest and most common way is to take the cross-sectional area of the conduit as the evaporation area (Figure 4a). However, the extended evaporating meniscus has larger surface area than the cross-sectional area, except in extremely small systems, where the adsorbed layer thickness is comparable with the system size. Therefore, this selection usually leads to an overestimation of heat fluxes. The second option is to take the extended meniscus area as the evaporation area (Figure 4b). The surface area of the meniscus extended between the adsorbed layers on the channel walls is calculated based on a curve fit (shown by solid blue line) to the liquid–vapor interface (shown by semitransparent blue line). The estimated extended meniscus area is slightly smaller than the cross-sectional area because of omission of the adsorbed layer. Another option is to take the liquid–vapor interfacial area including the adsorbed layer interface as the evaporation area (Figure 4c). The interfacial area of adsorbed layers on both channel walls is added to the extended meniscus area. Calculation of evaporation fluxes based on these area selections yields (a) 3379 kg s\(^{-1}\) m\(^{-2}\) for the cross-sectional area between the channel walls; (b) 3870 kg s\(^{-1}\) m\(^{-2}\) for the liquid meniscus area based on a curve fit to the liquid–vapor interface; and (c) 1414 kg s\(^{-1}\) m\(^{-2}\) for the total liquid–vapor interfacial area including the adsorbed layer interface. Moreover, an approximate upper bound for the evaporation is estimated based on the Hertz–Knudsen (H–K) equation\(^{21,22}\) (also known as the Hertz–Knudsen–Langmuir relation)

\[
m^* = \frac{M}{2\pi R^2} \left( \frac{R v}{\sigma_v} \right)^{1/2} \left( \frac{T_v}{T_{lv}} \right)^{1/4} \frac{1}{R v} \left( \frac{R v}{T_{lv}} \right) \]

where \(M\), \(R\), \(T_{lv}\), \(P_{lv}\), \(T_v\), \(P_v\), \(\sigma_v\), and \(\sigma_s\) are the molecular weight, universal gas constant, liquid–vapor interface temperature, vapor pressure just above the interface, vapor temperature, vapor pressure, evaporation coefficient, and condensation coefficient, respectively. While the first two area selections result in higher flux values, inclusion of the adsorbed layer renders the evaporation flux to a smaller value than the estimated upper bound (3235 kg s\(^{-1}\) m\(^{-2}\)) based on unit evaporation and condensation coefficients. Therefore, inclu-
sion of the adsorbed layer in the calculation of the effective evaporation area can drop the excessive evaporation fluxes reported in recent experiments\(^\text{44,25}\) below the kinetic limit calculated by these studies.

It should be pointed out that precise calculation of the kinetic limit depends on the proper selection of empirical parameters (evaporation and condensation coefficients), and these parameters were reported not to be bounded by unity based on the transition probability concept of quantum mechanics, called statistical rate theory (SRT).\(^\text{38}\) However, experimental studies were unable to measure the vapor pressure and temperature near the interface, which are necessary to calculate the coefficients in the modified H–K relation based on SRT

\[
\sigma = \frac{P_{ev,v}}{R_T} \exp \left[ (DOF + 4) \left( 1 - \frac{T_v}{T_l} \right) \right]^{DOF+4}
\]

\[
\sigma = \sqrt{\frac{T_v}{T_l}} \exp \left[ -(DOF + 4) \left( 1 - \frac{T_v}{T_l} \right) \right]^{DOF+4}
\]

where DOF is the vibrational frequency degrees of freedom, and three translational degrees of freedom are predicted for an ideal monatomic gas.\(^\text{39,40}\) The resultant coefficients (\(\sigma_l = 2.17\) and \(\sigma_v = 0.98\)) yield a much higher kinetic limit (10 \(414\) kg s\(^{-1}\) m\(^{-2}\)) for our first simulation, which demonstrates that proper calculation of evaporation and condensation coefficients is able to put a higher upper bound for the evaporation fluxes.

Although the missing physical connection (in the H–K equation) between the vapor and liquid phases during evaporation can be established by the utilization of SRT-based coefficients,\(^\text{48}\) the coupled nature of heat and mass transfer is still not considered,\(^\text{40,41}\) which makes both kinetic and statistical rate theories questionable in terms of putting an upper bound for the evaporation fluxes.

Figure 5. Sample simulation domain and its neighboring periodic images. Application of periodic boundary conditions in all directions is geometrically equivalent to the replication of the simulation domain throughout the space to form an infinite lattice. For the sake of brevity, we included only the neighbor images to a sample simulation domain in the figure. The center plane of each wall is actually a stagnation zone because of the merging of two opposite streams. This stagnation plane and the opposing streams are emphasized in the close-up view.

A massive body of literature exists for the theoretical modeling and experimentation of the evaporating meniscus in the continuum level.\(^\text{8–20}\) In these studies, the concept of disjoining pressure—suppression of the local film pressure due to the strong interaction between wall and liquid atoms—together with the capillary pressure were responsible for the pressure jump at the liquid–vapor interface. The variations of these pressures drove the liquid flow toward the contact line, where a planar adsorbed layer without any liquid flow is attached because of the vanishing capillary and disjoining pressure gradients. The absence of lateral momentum transport confirmed the equilibrated adsorbed layer with zero net evaporation in previous studies. However, origin of the strong passive flow adjacent to a solid wall with a substantial temperature gradient is the variation of the solid–liquid surface tension,\(^\text{37}\) and the lateral mass flow in a constant thickness layer requires the same amount of evaporation to conserve the mass as shown in Figure 3. Previous experiments\(^\text{26–16}\) carried out under near isothermal or slight heating conditions, were unable to show the evaporation from adsorbed layers because of the insufficient thermal gradient of the solid substrate.

### CONCLUSIONS

Our computational experiments demonstrated that adsorbed liquid films attached to liquid–vapor interfaces are able to turn sharp corners, transport momentum, and evaporate. Although the amount of liquid evaporating from the adsorbed layers is negligible for macroscopic systems, this amount is comparable to the total evaporation for systems having a few nanometers.

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\[ A = \frac{\pi r^2}{2} \]
or sub-nanometer interfaces. Therefore, precise calculation of evaporation rates on these scales requires atomic modeling of liquid–vapor interfaces. Our computational setup allows steady-state evaporating and condensing liquid–vapor interfaces located in capillary nanoconduits, making it a useful tool for investigating phase-change processes on the nanoscale.

ASSOCIATED CONTENT

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.langmuir.8b04219.

Details of MD simulations; mass flow through adsorbed region; uncertainty analysis; location and profile of the evaporating meniscus for different heating loads; and flow and temperature fields (PDF)

Demonstration of the lateral momentum transport within and evaporation from the adsorbed layer (AVI)

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Notes
The authors declare no competing financial interest.

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