Prediction of heat and mass transport in micropillar wick evaporators with Marangoni convection

Goksel Yuncu\textsuperscript{a,b}, Yigit Akkus\textsuperscript{a}, Zafer Dursunkaya\textsuperscript{b}

\textsuperscript{a}ASELSAN Inc., 06200 Yenimahalle, Ankara, Turkey
\textsuperscript{b}Department of Mechanical Engineering, Middle East Technical University, 06800 Çankaya, Ankara, Turkey

Abstract

Thin-film evaporation and the replenishing capillary liquid flow have paramount importance for various technological applications spanning from desalination to electronics cooling. With the developments enabling faster and cheaper yet more precise fabrication, evaporators with micropillar arrays have attracted substantial attention to sustain efficient evaporation fed by passive liquid transport. Although considerable effort has been devoted to designing optimized wicks, the full picture is still blurry due to complexities in modeling the liquid-vapor interface and the flow around the micropillars. Fundamentally, the heat transfer from a micropillar wick evaporator is a problem governed by various interfacial phenomena such as the capillarity induced liquid flow, thin-film evaporation intensifying near the contact lines, and thermocapillarity induced Marangoni flow. However, past works have not been able to assess the effect Marangoni flow due to the missing coupling between cell- and device-level modeling. In this work, we develop a comprehensive model for the evaporation from a micropillar wick evaporator by coupling the liquid flow with the energy transfer in both liquid and solid domains at both cell- and device-levels. The model is successfully validated with previous experiments. When Ma number is sufficiently high, the model identifies a sharp reduction in the evaporator temperature attributed to the thermocapillary convection creating circulations beneath the liquid-vapor interface. This temperature reduction cannot be identified when thermocapillarity is switched off in the model and the model’s prediction substantially deviates from the experimental measurement. Therefore, the current study reveals a hitherto unexplored role of Marangoni flow in the evaporation of water from micropillar wick evaporators. We believe that the proposed modeling framework can guide the engineers for the optimization of micro-post evaporators by accounting for all the relevant interfacial phenomena.

Keywords: thin-film evaporation, capillary flow, Marangoni flow, micropillar wick, dry-out heat flux.
1 Introduction

Continuous improvements in semi-conductor fabrication techniques open up an avenue for the production of integrated circuits with increasing computational power in the past decades. While the decrease of feature size on a 2D chip had determined the performance in conjunction with the Moore’s law [1]; now, in the post-Moore era, performance is still enhanced by stacking 3D chips vertically. Yet, all these progress come with an inevitable cost: excessive heat fluxes. Specifically, excessive local heat fluxes (e.g. power amplifier hot spots exceeding $10 \text{ kW cm}^{-2}$ heat flux [2]) create drastic thermal challenges, which are impossible to be handled by traditional approaches. These hot spots may be actively cooled down in situ by intra-chip liquid circulation by establishing proper microfluidics-based solutions [2]. When intra-chip active liquid cooling could not be established, the heat from the hot spots should be transported to a wider heat removal area with a sufficiently small thermal resistance to eliminate the excessive temperature rise.

When conduction is the sole energy transport mechanism, thermal resistance is determined by the thermal conductivity of the solid, which is inadequate to materialize the desired resistance values. This issue can be overcome by two-phase heat spreaders using the liquid-vapor phase change as the energy transport mechanism. The bottleneck in the design of two-phase heat spreaders is the evaporator due to the need for removing localized heat inputs of excessively large magnitudes without any dryout. The design success is determined based on the optimization of the wick structure, which should provide sufficient liquid pumping together with minimum film resistance. A thorough optimization demands control over both the design parameters and fabrication. Owing to the advances in micro and nano fabrication techniques, the high-resolution control of surface topography over length scales ranging from molecular-level to macro-level becomes possible, which allows numerous opportunities for the heat transfer enhancement via varying scale surface structures [3–5]. As opposed to the coating-based methods (e.g. nanowire coating, CNT coating, etc.), which, in general, generate a random distribution of surface features, lithography-based methods are able to create features (e.g. micro-scale and nano-scale posts, etc.) with exact shapes and sizes. Accordingly, thin-film evaporation from these engineered surfaces has gained substantial attention in recent decades.

Evaporators with micro-scale posts (commonly referred to as micropillars) have been extensively studied both experimentally [6–8] and numerically [9–11]. Cylindrical micropillars attracted substantial attention among the different shaped micro-post evaporators due to their superior capillary pressure and permeability performance compared to their polygon-shaped counterparts with sharp corners [9]. The performance of an evaporator is assessed by the maximum dryout heat flux and the effective thermal resistance of the wick structure [12]. While the maximum dryout heat flux is proportional to the capillary pressure and permeability, thermal resistance scales down with the interfacial area and up with the film thickness. Therefore,
accurate prediction of permeability, capillary pressure, and thermal resistance is essential for exploiting the full potential of an evaporator.

Many prior studies focused on the modeling of capillary liquid flow through the micropillar arrays without thermal considerations. A common simplification was to assume a 2-D liquid flow through square and hexagonal packed arrays of infinitely long micropillars [13–17]. The effect of interfacial geometry (i.e., 3-D meniscus shape) was also negated in previous capillary flow models [18–20]. These models primarily characterized the flow in terms of effective porosity and permeability that were obtained via Darcy’s law [15–18] or Brinkman equation [19, 20].

Because of its 3-D nature, meniscus shaped liquid-vapor interface established between the pillars cannot be straightforwardly determined. Surface Evolver [21], on the other hand, enables obtaining 3-D interfacial geometries based on the surface energy minimization principle. Many studies [7–9, 22, 23] utilized Surface Evolver to generate the interfacial geometry a priori. They then calculated the permeability and thermal resistance accordingly as inputs for the numerical simulations. These studies revealed that the increase in interface curvature enhances the evaporation flux by widening the thin-film region, whereas it deteriorates the liquid flow by reducing the wick permeability due to decreasing flow area [9, 22]. The accuracy of different permeability models [8, 9, 15, 16, 23] is experimentally and theoretically assessed on four different wick structures by Ravi et al. [10]. They suggested a unified model that can predict the mass transfer with an error less than 18% by combining the capillarity model of [8] and the permeability model of [23]. For the better prediction of dryout heat flux, Zhu et al. [11] developed a model by considering the variation of the meniscus shape with capillary pressure and local permeability. They also conducted validation studies by experimenting evaporation into air atmosphere and reported the optimal wick geometry for the maximum dryout heat flux as functions of pillar diameter ($d$), height ($h$), and the pitch ($l$) as follows: $d/h \sim 0.4 - 0.6$ and $l/d \sim 3.0$.

In addition to the studies targeting the prediction of dryout heat load, there were other works [9, 28–32] that focused on the estimation of interfacial heat flux by considering the thin-film evaporation and/or applying kinetic theory based evaporation models. Ranjan et al. [28] investigated the wicking performance and effective thermal resistance for commonly used topologies as a function of a non-dimensional number that defines the characteristics of microstructures, liquid filling volume, and the contact angle. Farokhnia et al. [30] conducted theoretical and experimental studies to systematically optimize interfacial heat flux for rectangular ribs, vertical circular, and square pillar configurations. They determined evaporative mass flux at the interface using Hertz-Knudsen equation and suggested an optimum pitch-to-diameter ratio, $l/d \sim 1.8$, to maximize the heat flux by thin-film evaporation. Recently, Bongarala et al. [32] developed a non-dimensional metric (a figure of merit) to evaluate the evaporative heat flux for several wick structures and compared their predictions with those in previous works [9, 29, 31].
More comprehensive models were developed by coupling the fluid flow and thermal models to investigate the evaporation from cylindrical micropillars. Adera et al. [33] investigated the effect of porosity and pillar height for the optimum wick design to maximize the evaporation performance. They predicted the dryout heat flux based on a semi-analytical model similar to that of [23] and estimated the interfacial thermal resistance using Schrage equation [34]. The authors employed invariant permeability and thermal resistance values at the receding contact angle for the entire domain and neglected the curvature variation along the wicking direction. They also conducted verification experiments under a controlled environment sustaining steady evaporation into pure vapor and validated their model with 20% accuracy. Wei et al. [35] carried out a parametric investigation to optimize the wick design by conducting a wide range of experiments using varying micropillar geometries. In addition, the authors assessed their experimental results, specifically dryout heat flux and superheat, based on previous modeling efforts [10]. Somasundaram et al. [36] compared the accuracy of existing permeability models and provided guidance for the optimal design to maximize dryout heat flux and minimize thermal resistance simultaneously. Recently, Vaarstra et al. [12] developed a comprehensive model to apprehend arbitrary thermal load and non-uniform evaporation by extending the permeability model of [11]. The model accurately calculates the variation of the capillary pressure, heat transfer coefficient and temperature distribution along the substrate.

Fundamentally, the heat transfer from a micropillar wick evaporator is a problem governed by various interfacial phenomena such as the capillarity induced liquid flow or thin-film evaporation intensifying near the contact lines. Thermocapillarity is also a well-known mechanism, which induces a surface flow (commonly known as Marangoni flow) on non-isothermal interfaces. Its significant contribution to the convective transport, and the heat transfer thereof, was experimentally and theoretically demonstrated in different systems such as the evaporation of water droplets [37–39]. However, the role of Marangoni convection in the micropillar wick evaporators has been overlooked mostly due to the complexity of the modeling for this problem. In fact, there were early modeling efforts to assess the effect of Marangoni flow in micropillar wicks [9, 29]. However, these attempts were not able to address the true effect of thermocapillarity since the transport mechanisms were handled only at the cell-level, which prevented exploring its impact on the capillary flow along the substrate, and the overall thermal performance thereof.

In the present study, we aim to build a comprehensive model for simultaneous prediction of dryout heat flux and local temperature distribution for a micropillar wick evaporator. We extended the permeability and thermal resistance model developed in [11, 12] to capture the effect of thermocapillarity induced Marangoni convection in the cell-level model. The effect of Marangoni convection is then reflected on the device-level model in terms of permeability and effective thermal resistance for evaporation. The current model is validated with three
controlled sets of distinct experiments to exhibit the model’s capabilities in predicting dryout heat flux, heat transfer coefficient, and the effect of Marangoni flow.

2 Methodology

The evaporation from regularly packed pillar arrays is investigated at the micro (cell-level) and macro (device-level) scales to obtain sufficiently accurate results with a low computational cost. First, parametric studies are performed at the cell-level for a wide range of geometries and contact angles to obtain curvature-dependent permeability ($\kappa$) and effective heat transfer coefficient ($h_{eff}$) as a function of geometry and capillary pressure. Then curvature-dependent local permeability and heat transfer coefficient values are utilized in the discretized device-level model, where all cells are linked to satisfy the conservation of mass, momentum, and energy throughout the substrate by coupling the energy and fluid transport problems. Dryout heat flux, local heat transfer coefficients, and temperature distribution on the substrate are acquired for an arbitrary thermal load applied at the bottom of the substrate.

2.1 Cell-level Model

In the cell-level model, initially, 3-D meniscus shapes at various contact angles are generated (Sec. 2.1.1). Then the generated 3-D geometries are employed as the computational domain for cell-level energy (Sec. 2.1.2) and liquid (Sec. 2.1.3) transport problems together with the thermocapillarity induced flow (Sec. 2.1.4).

2.1.1 Meniscus Shape

Three-dimensional meniscus shape established between the pillars is a function of the local liquid pressure and vapor pressure. Assuming negligible variation of the vapor pressure, capillary pressure, $\Delta p_c$, is defined as the local liquid-vapor pressure difference $\Delta p_c(x) = p_v - p_l(x)$ that is calculated by the Young-Laplace (Y-L) equation:

$$\nabla \cdot \hat{n} = \Delta p_c(x)/\sigma$$

(2.1)

where $\sigma$ is surface tension, and $\hat{n}$ is the outward unit normal of the surface. The shape of interface is denoted as a geometric function of the surface height, $H$, and the unit outward normal of the interface is defined as follows:

$$\hat{n} = \frac{(H_x, H_y, -1)}{(H_x^2 + H_y^2 + 1)^{1/2}}$$

(2.2)

After substituting Eq. (2.2) into Y-L equation, appropriate boundary conditions are needed to
solve this nonlinear differential equation. By taking the advantage of the symmetries within a unit-cell, only a quarter of the unit-cell is accounted as the problem domain (Fig. 1b). The three-phase contact line is fully pinned to the pillar top \((z=0)\), and the other boundary conditions are defined as symmetry conditions. Then the Y-L equation is solved to obtain the 3-D meniscus shape for a given capillary pressure and geometry. The generated 3-D liquid domain serves as the simulation domain for liquid and energy transport problems in the cell-level model. In order to accurately capture the effect of the interface variation in the wicking direction, a sweep solution for various contact angles is conducted between the flat \((\theta=90^{\circ})\) and fully stretched menisci \((\theta=\theta_{rec})\). The relation between the liquid-vapor pressure difference and contact angle is obtained by the force balance as follows:

\[
\Delta p_c(\theta) = \frac{4\sigma \cos(\theta)}{d \left[ \frac{4}{\pi} \left( \frac{l}{d} \right)^2 - 1 \right]}
\]

where \(\theta\) is the contact angle, \(l\) is the pitch, and \(d\) is the diameter of the pillar. The accuracy of the Y-L equation solutions is ensured by comparing the 3-D meniscus shapes obtained from the simulations with those measured in the study of Adera et al. [33] in the Supporting Information.

![Figure 1](image-url)

**Figure 1:** a) Top view of the evaporator. The pillar array dimensions are \(d, l, h,\) and \(L\), where \(d\) is diameter, \(l\) is pitch, \(h\) is height, \(L\) is the total wicking length. b) Top and front view of the quarter unit-cell and boundary conditions for the heat transfer problem. c) Top and front view of the half unit-cell and boundary conditions for the flow problem.

### 2.1.2 Energy Transport

Cell-level thermal model aims to obtain the effective heat transfer coefficient, \(h_{eff}\), as a function of capillary pressure and geometric dimensions. The effective heat transfer coefficient serves as an input for the device-level model and it is defined in terms of the applied heat flux, \(q''_e\), and the average evaporator superheat, \(\Delta T\), as follows: \(h_{eff} = q''_e / \Delta T\), where the average evaporator


superheat is the difference between average evaporator temperature, $T_{e, av}$ (see Fig. 1b) and the vapor temperature, $T_v$: $\Delta T = T_{e, av} - T_v$. To obtain $T_{e, av}$, temperature distribution at the liquid-substrate interface needs to be found, which is calculated by solving the heat transfer problem at the cell-level.

Slow liquid propagation (small Reynolds number) and resulting low evaporation enable decoupling the liquid flow and heat transfer. While the flow modeling does not require including evaporation rate from the meniscus (no shear boundary conditions is appropriate), the thermal model can be solved with stationary fluid domain assumption since the conduction dominates the convective energy transport within the fluid. Accordingly, steady-state heat equation is solved for the energy transport. The same symmetry conditions utilized in the solution of Y-L equation are valid for the thermal model, which is also solved in the quarter unit-cell domain (Fig. 1b). Uniform heat flux is applied at the bottom of the substrate to include the construction resistance of the substrate base [40]. Pillar top is assumed insulated due to the negligible energy transfer via natural convection. Utilizing kinetic theory of gases, evaporative mass flux can be calculated based on the interfacial properties of the vapor and liquid. When the evaporation rate is not excessive, Schrage’s original expression [34] reduces to an approximate form [41]:

$$\dot{m}_{evap}'' = \frac{2\hat{\sigma}}{\hat{\sigma}} \left( \frac{M}{2\pi R_u} \right)^{1/2} \left( \frac{p_{sat}|T_{lu}}{T_{lu}^{1/2}} - \frac{p_v}{T_v^{1/2}} \right)$$  (2.4)

where $\hat{\sigma}$, $M$, $R_u$, $T_{lu}$, $p_{sat}|T_{lu}$, $T_v$, and $p_v$ are the mass accommodation coefficient, molar mass of the liquid, universal gas constant, interface temperature, saturation pressure at the interface temperature, vapor temperature, and vapor pressure, respectively. Evaporative mass flux is imposed onto the meniscus as the interfacial heat transfer coefficient ($h_{int}$) to imitate the heat loss from the meniscus via evaporation:

$$h_{int} = \dot{m}_{evap}'' \left( \frac{h_{fg}}{T_{lu} - T_v} \right)$$  (2.5)

where $h_{fg}$ is the latent heat of vaporization of the liquid. Applying this interfacial heat transfer coefficient together with other aforementioned boundary conditions, the governing equation ($\nabla^2 T = 0$) is solved using FEM solver of COMSOL Multiphysics software [42]. The effect of heat flux on the evaporation resistance is investigated by conducting the parametric studies with various heat fluxes.

### 2.1.3 Liquid Transport

Cell-level flow model aims to obtain the liquid permeability, $\kappa$, of the pillar structure in the wicking direction. Permeability serves as an input for the device-level model and it can be calculated based on the Darcy’s law. To obtain $\kappa$, liquid flow is solved in the half unit-cell
Evaporative mass flow is neglected, since evaporation induced liquid velocity perpendicular to the meniscus is low ($Re_z \ll 1$). No shear boundary condition on the meniscus (viscosity of vapor is very low to cause friction on the interface), symmetry on the sides, no-slip boundary condition on the solid surface, and periodic boundary condition with a pressure difference between the inlet and outlet of the domain are applied to ensure fully developed liquid flow. With these boundary conditions, Navier-Stokes equations are solved using the FEM solver of COMSOL Multiphysics. Then the resultant flow rate is utilized to back-calculate the permeability, $\kappa$, from Darcy’s law:

$$\bar{U} = \frac{1}{A_c} \iint u \, dy \, dz = -\frac{\kappa}{\mu} \nabla p$$

(2.6)

where $\bar{U}$ is the average velocity, $u$ is the velocity component in the $x$-direction, $A_c$ is the cross-sectional area at the outlet, $\mu$ is dynamic viscosity which is temperature dependant, and $\nabla p$ is the applied pressure difference over a pitch of the pillar array. For a set of given pillar array dimensions, the capillary pressure defines the curvature of the interface, and dynamic viscosity is a function of temperature; therefore, permeability ($\kappa$) is a function of local pressure and temperature. Solving permeability for various $\theta$ provides the relation between local permeability and capillary pressure. For simplicity, we conduct parametric simulations with a reference temperature of the liquid equal to the vapor temperature. However, in the device-level simulations, permeability is modified as a function of the average liquid temperature that increases due to the applied heat flux.

### 2.1.4 Thermocapillary Flow

Thermocapillary flow is driven by the surface tension variation on the liquid-vapor interface originating from the temperature gradients. The impact of thermocapillary flow can be measured with the Marangoni number, which is defined as: $Ma = (\partial \sigma / \partial T) \left(L_t \Delta T_{int} / \mu \alpha \right)$, where $L_t$ is the length scale of the domain (tangential distance on the meniscus between the pillar edge and a corner of the unit-cell), $\Delta T_{int}$ is the maximum temperature difference at the interface, and $\alpha$ is thermal diffusivity of the liquid. Accordingly, in the case of high superheat and/or large pitch, thermocapillary flow can trigger an effective internal convection in a cell.

The half unit-cell (see Fig. [c]) is considered as the simulation domain for the multi-physics problem, where cell-level flow and thermal models are coupled. To account for the thermocapillary driven convective energy transport, full steady state energy equation (with convective terms) is utilized: $\rho c_p u \cdot \nabla T = \nabla \cdot (k \nabla T)$. Regarding boundary conditions, surface normal gradients of temperature and velocity are set to zero at the sides due to the symmetry condition. In addition to periodic flow boundary condition shown in Fig. [c], thermal periodic boundary
condition (without temperature difference) is applied at inlet and outlet surfaces. Tangential force balance is applied between the thermocapillary and the shear force associated with the liquid at the liquid-vapor interface as follows: 

$$-\hat{n} \cdot \bar{\tau} \cdot \hat{t} = \nabla \sigma \cdot \hat{t},$$

where $\bar{\tau}$ is the deviatoric stress tensor defined as $\mu (\partial u_i / \partial x_j + \partial u_j / \partial x_i)$ and $\hat{t}$ is the unit tangential vector. With these boundary conditions, governing equations are simultaneously solved using the FEM solver of COMSOL Multiphysics. Thereafter, permeability ($\kappa$) and heat transfer coefficients ($h_{eff}$) at various heat fluxes are stored to create lookup tables for a given geometry. Parametric simulations are performed at different contact angles and heat fluxes for a wide range of pillar array dimensions to observe the impact of the thermocapillary flow in the device-level model.

### 2.2 Device-level Model

In the device-level model, evaporation is compensated by replenishing flow, which is driven by the variance of the capillary pressure along the wicking direction. The liquid replenishing is maintained until the contact angle of the meniscus in a unit-cell reaches the receding contact angle, which is herein denominated as the receding onset, and the corresponding heat flux is called dryout heat flux for a given pillar array dimensions.

In the model, a heat input, $q''_m(x)$, is applied at the bottom surface of the substrate with a base thickness of $t_s$ (see Fig. 2). For the energy transfer mechanism from the heated micropillar substrate to the ambient, only evaporative heat transfer is accounted for. The device-level model is established based on the flow (see Fig. 2a) and conduction (see Fig. 2b) domains, which are discretized in accordance with the unit-cells utilized in the cell-level modeling. Then all cells are linked to satisfy the conservation of mass, momentum, and energy by an outer iterative loop to imitate the thin-film evaporation from a regularly packed pillar array evaporator.

First, the flow domain (Fig. 2a) is considered to obtain the capillary pressure variation along the wicking direction for a predefined heat flux. The capillary pressure and mass flux at the inlet are sufficient to acquire capillary pressure distribution over the entire domain since the pressure drop depends on permeability ($\kappa$) and mass flow rate ($\rho A \bar{U}$) according to Darcy’s law. Since the applied heat flux is removed solely by the evaporation, the corresponding total liquid mass flux is calculated as the inlet boundary condition, and the capillary pressure-dependent permeability values for each cell are obtained from the lookup tables generated \textit{a priori}.

After the calculation of $\Delta p_c(x)$ along the flow domain, the spatial distribution of $h_{eff}$ is obtained and utilized in the device-level conduction domain (Fig. 2b). In the first iteration, $\Delta p_c(x)$ is calculated by neglecting the axial conduction in the substrate. However, the applied heat flux at the bottom of the substrate results in nonuniform evaporation through the axial conduction due to the spatial variation of $h_{eff}$. Conduction and flow domains are solved iteratively by an outer loop till the convergence. The computational scheme of the developed model and mesh independence study are presented in the Supporting Information.
Figure 2: Representation of the device-level model for thin-film evaporation. In the device-level simulations, local capillary pressures, average fluid temperature, and temperature distributions on the substrate are calculated. 

a) In the device-level flow model; pressure distribution along the wicking direction is calculated by Darcy’s law and former lookup tables. Each unit-cell has a meniscus with different curvature, and capillary pressure thereof. 

b) In the device-level conduction model; capillary pressure dependent effective heat transfer coefficient is assigned at the top surface of the substrate base, and an arbitrary heat flux is applied at the bottom of each unit-cell. Heat transfer through the side walls is assumed negligible.

3 Results and Discussion

The current model is validated against three distinct sets of experiments conducted in previous studies [11, 33, 35], where all substrates were made of silicon with a wide variety of pillar dimensions and the working liquid was deionized water. Varying heat inputs were applied under different ambient conditions. The substrates with similar pillar dimensions led to near predictions for the dryout heat flux or superheat values. Accordingly, selected cases from these studies (see Table 1) are included in the validation of the model for brevity. For all experiments, pillar dimensions were sufficiently small to prevent the boiling incipience.

In the first experimental work [11] simulated by the proposed model, evaporation took place into the air from two different samples (Device-A1 and Device-A3 in Table 1). While the pillar diameter and height were close, pitches of the pillars were different (20 µm vs. 50 µm) in these substrates. Accordingly, the wicking ability of the substrates differs substantially. In the experiments, the substrate with the denser pillar forest could withstand a higher heat load.
Table 1: Details of the micropillar wick evaporators and experimental conditions in previous experiments \cite{11,33,35}, which are simulated by the proposed model.

| Device ID | d (µm) | w (µm) | h (µm) | \(\theta_{rec}\) (°) | \(T_{sat}\) (°C) | \(q''_{in}\) (W cm\(^{-2}\)) | \(\Delta T_{int}\) (°C) | Ma |
|-----------|-------|-------|-------|----------------|-----------------|----------------|----------------|---|
| Device-A1 \cite{11} | 7 | 20 | 20 | 15 | 100* | 0–47 | - | - |
| Device-A3 \cite{11} | 6 | 50 | 19 | 15 | 100* | 0–27 | - | - |
| Device-1 \cite{33} | 5 | 12 | 82 | 70 | 24 | 0–46 | 3.0 | 21 |
| Device-5 \cite{33} | 12 | 20 | 90 | 70 | 24 | 0–45 | 4.3 | 62 |
| Sample-1 \cite{35} | 23.4 | 41.0 | 39.5 | 10 | 25 | 0–28 | 1.9 | 48 |
| Sample-2 \cite{35} | 25.9 | 41.0 | 39.5 | 10 | 25 | 0–22 | 1.5 | 33 |
| Sample-3 \cite{35} | 28.2 | 41.0 | 39.5 | 10 | 25 | 0–23 | 1.1 | 24 |
| Sample-4 \cite{35} | 22.1 | 41.0 | 39.5 | 10 | 25 | 0–23 | 2.1 | 52 |
| Sample-5 \cite{35} | 23.4 | 36.0 | 39.5 | 10 | 25 | 0–22 | 1.1 | 21 |
| Sample-6 \cite{35} | 23.4 | 34.0 | 39.5 | 10 | 25 | 0–20 | 0.8 | 15 |
| Sample-7 \cite{35} | 23.4 | 44.0 | 39.5 | 10 | 25 | 0–25 | 2.4 | 64 |
| Sample-8 \cite{35} | 23.2 | 41.0 | 79.7 | 10 | 25 | 0–60 | 7.0 | 216 |

* Evaporation into the air environment at 1 atm.

without drying for the same liquid wicking length. The predictions of the proposed model excellently match with the experimental measurements as shown in Fig. 3 where maximum wicking lengths at the onset of dryout are presented for different heat fluxes. While this comparison reflects the success of the proposed model in terms of liquid transport, the sensitivity of the model to the thermal effects could not be assessed since no temperature data were available.

Secondly, the experimental work of Adera et al. \cite{33} is utilized to verify the thermal capabilities of the proposed model. In their experiments, the evaporation took place into a controlled environment with pure vapor and the wicks were in contact with the liquid at the four sides of the substrate. Accordingly, bi-directional liquid flow is considered in our modeling to represent the physics accurately (see the Supporting Information for the details of bi-directional flow modeling). A relatively high receding contact angle (\(\theta_{rec} = 70°\)) was observed in the experiments, which was attributed to the presence of polymer remaining on the pillars. The temperature of the substrate was measured at different heat fluxes by gradually increasing the applied heat input, and the average temperature at the evaporator was estimated through a one-dimensional thermal resistance model. These average evaporator temperature estimations of Adera et al. \cite{33} are successfully predicted by the proposed model as shown in Fig. 4 where the average temperature is represented by the average evaporator superheat.
Figure 3: Comparison of the dryout heat flux predictions of the proposed model and the experimental results of Zhu et al. [11].

Figure 4: Comparison of the average evaporator superheat predictions of the proposed model and the experimental results of Adera et al. [33]. For both devices, MAC value of 0.06 is utilized in the estimation of evaporation rates.

It should be noted that evaporator temperature is primarily dictated by the rate of evaporation, which determines the extent of the evaporative cooling. Therefore, calculation of the evaporation rate via Schrage’s approximate expression (Eq. (2.4)) has a great importance for
the prediction of temperature in our model. However, Schrage’s expression includes a parameter, \( \hat{\sigma} \), called mass accommodation coefficient or MAC in short, which does not possess a common universal value. In fact, it is a system-dependent parameter \[36\], which varies with the type of the liquid, system cleanliness, etc. From the kinetic theory point of view, a departure from the equilibrium alters the macroscopic vapor (drift) velocity and the thermophysical properties in the vapor. These effects influence the value of MAC utilized in the estimation of evaporation, since evaporation is inherently a phenomenon shifting the equilibrium. Further discussion is out of the scope of this study, thus we kindly refer the reader to past works focusing on MAC \[43\] or evaporation/condensation coefficients in a broader perspective \[44\]. Our strategy in the current work was to determine a MAC value for each device and utilize this value for the experiments conducted on the same device. With this approach, a system-specific MAC is obtained, which enables accounting for the uncontrollable parameters associated with the experimentation. We, however, refrain from assigning different MAC values to each experiment, since it would not be practical when modeling is performed for design purposes and it might break the connection between MAC and the system by turning MAC into a fudge factor serving as a fitting parameter between each simulation and experiment.

Induction of a Marangoni flow on the water interface can be hindered due to the presence of a small amount of contamination \[45\]. The presence of polymer remaining on the pillars fabricated for the study of Adehra et al. \[33\] makes those experiments inappropriate for the investigation of the effect of thermocapillary flow on the evaporation from micropillar evaporators. On the other hand, the study of Wei et al. \[35\] provides a suitable base for the investigation of thermocapillary flow by providing a set of evaporation experiments into pure vapor environment across a wide range of Ma numbers (see Table 1). Moreover, the observation of a low receding contact angle of the water \( (\theta_{\text{rec}} = 10^\circ) \) suggests contamination-free pillars. Therefore, the current model is applied to simulate the experiments of Wei et al. \[35\]. The modeling is made for three different scenarios to assess the individual effects of temperature variation and Marangoni flow: i) isothermal model, ii) non-isothermal model, and iii) Marangoni model. In the isothermal model, the liquid temperature is set to the vapor temperature and the liquid temperature increase associated with the applied heat load is neglected. But this simplification directly affects the thermophysical properties, especially the liquid viscosity, which is appreciably sensitive to the temperature. In the non-isothermal model, on the other hand, the liquid temperature increase is obtained from the cell-level thermal model and the modeling is performed based on temperature-dependent thermophysical properties. In the Marangoni model, thermocapillary convection is also included such that all active transport mechanisms are taken into consideration in the model.

The first comparison is made for the dryout heat fluxes as shown in Fig. 5a. Since the temperature rise is relatively restricted for the first seven samples, predictions of isothermal
Micropillar wick evaporators with Marangoni convection

Yuncu et al.

and non-isothermal models are close. However, for Sample-8, which has the highest heat input, the isothermal model fails to correctly predict the dryout heat flux due to the omission of thermal effects. A similar trend is also noticed for the Marangoni model. Moderate variation of interfacial temperature keeps Ma number relatively small (see Table 1), which leads to almost identical results for non-isothermal and Marangoni models in the first seven samples. Yet, for Sample-8, there is a slight deviation between the dryout heat flux predictions of non-isothermal and Marangoni models. Moreover, the prediction of Marangoni model is closer to the experimental result, which gives a clue for the effect of thermocapillary convection. However, this slight difference prevents us from making a strong conclusion. Then the second comparison is made, now, for the average evaporator superheats as shown in Fig. 5b. At this time, the isolated effect of thermocapillary convection is apparent. For Sample-8, the non-isothermal model fails to predict the average evaporator superheat, whereas the Marangoni model successfully predicts it.

Figure 5: Comparison of the a) dryout heat flux and b) average evaporator superheat predictions of the proposed model and the experimental results of Wei et al. [35]. Different MAC values between 0.1 and 0.4 are assigned to each sample and the assigned value is utilized for all experiments conducted on the corresponding sample in the estimation of evaporation rates.

Since the average temperature of Sample-8 is substantially affected by thermocapillarity, Marangoni convection is expected to widely shape the liquid flow near the liquid-vapor interface. To reveal this, liquid flow patterns at different cross-sections of a unit-cell parallel to the wicking direction are presented in Fig. 6 for Sample-8. As shown in all cross-sections, thermocapillarity induces surface flows leading to circulations in a varying extent. While these surface flows are in the same direction with the wicking (capillary) flow at the downstream-half of a unit-cell, they oppose the wicking flow at the upstream-half of a unit-cell. The origin of these thermocapillary surface flows is the interfacial temperature variation. Resultant temperature distributions on
the interface (top view) together with different cross-sections parallel to the wicking direction are provided in Fig. 7. As shown in the top view, a thermal boundary layer with a significant temperature gradient develops on the liquid-vapor interface near the pillar contact line. This temperature gradient triggers a radially outward surface flow from the warmer pillar contact line to the cooler zones around the pillar leading to the flow patterns shown in Fig. 6.

Figure 6: Magnitude of the velocity component in the wicking ($x$-) direction with superimposed streamlines at different cross-sections of a unit-cell parallel to the wicking direction. Positions of cross-sections are (as specified in the top view): a) at the pillar center, b) at the pillar edge, and c) at the symmetry center between adjacent unit-cells. Results are given for the Sample-8 experimented in Ref. [35] at the heat load of $q''_m = 50$ W cm$^{-2}$ for a unit-cell with the contact angle of $\theta = 30^\circ$.

The formation of periodic reverse surface flows is expected to decrease the mass transport in the wicking direction. Accordingly, the dryout heat flux is expected to decrease due to the associated capillary flow deficit. The extent of the deficit, on the other hand, scales down with the pillar height since the permeability of a wick with substantially long pillars is slightly affected by the dynamics of the surface flows. The capillary flow through the pillars of Sample-8, for instance, exhibits an undisturbed parallel flow pattern in the wicking direction except for a restricted near interface zone affected by the thermocapillarity, which penetrates through the liquid film no more than a quarter of the pillar height (see Fig. 6b-c). Therefore, dryout
Micropillar wick evaporators with Marangoni convection

Figure 7: Temperature field and superimposed total energy flux streamlines on the interface (top view), pillar center plane (view A-A), and symmetry center plane between adjacent unit-cells (view B-B). In view B-B, the liquid-vapor interface is shown by white solid line. Results are given for the Sample-8 experimented in Ref. [35] at the heat load of $q''_\text{in} = 50 \text{ W cm}^{-2}$ for a unit-cell with the contact angle of $\theta = 30^\circ$.

heat flux is slightly affected by the presence of Marangoni flow in Sample-8. On the other hand, thermocapillary flow significantly enhances the convective energy transport. As it can be seen in Fig. 7, energy transport paths follow the velocity streamlines by manifesting the convection as the primary energy transport mechanism. The warmer liquid is moved away from the pillar contact line with the surface flow so that cooler fresh liquid from the outer region replenishes it. The resultant circulation creates an effective mixing mechanism, which enhances the evaporation and the associated interfacial heat transfer coefficient. Accordingly, average evaporator temperature significantly reduces (ca. 5 °C) in the presence of Marangoni convection compared to the evaporation with the stationary liquid assumption.
4 Conclusion

Evaporation from a micropillar wick evaporator is modeled by coupling the capillary liquid flow with the energy transfer in both liquid and solid domains. Thermocapillary flow is accounted for in the modeling for the first time in the literature. Predictions of the model are compared with a wide range of previous experimental results for water evaporation from micropillar evaporators and excellent agreements are obtained. For the cases, where Ma number is relatively smaller, the effect of thermocapillarity on both dryout heat flux and average evaporator temperature is slight. However, when Ma number is sufficiently high, thermocapillary convection sharply decreases the evaporator temperature by creating circulations beneath the liquid-vapor interface. This temperature reduction cannot be identified when thermocapillarity is not accounted for in the modeling. Therefore, the current study successfully reveals the role of Marangoni flow in the evaporation of water from micropillar wick evaporators. We believe that our modeling approach can help researchers explore the relevant interfacial phenomena in the evaporation from the arrays of micro-scale surface structures and guide the engineers for the optimization of micro-post evaporators.

References

[1] G. E. Moore. Cramming more components onto integrated circuits. Electronics, 38(8):114, 1965.

[2] A. Bar-Cohen, M. Asheghi, T. J. Chainer, S. V. Garimella, K. Goodson, C. Gorle, and Y. Joshi. The icecool fundamentals effort on evaporative cooling of microelectronics. IEEE Trans. Compon. Packaging Manuf. Technol., 11(10):1546–1564, 2021.

[3] D. Li, G. S. Wu, W. Wang, D. Wang, Y. D. and Liu, D. C. Zhang, Y. F. Chen, G. P. Peterson, and R. Yang. Enhancing flow boiling heat transfer in microchannels for thermal management with monolithically-integrated silicon nanowires. Nano Lett., 12(7):3385–3390, 2012.

[4] D. Attinger, C. Frankiewicz, A. R. Betz, T.M. Schutzius, R. Ganguly, A. Das, C. J. Kim, and C. M. Megaridis. Surface engineering for phase change heat transfer: A review. MRS Energy & Sustainability, 1, 2014.

[5] Y. Akkus, C. T. Nguyen, A. T. Celebi, and A. Beskok. A first look at the performance of nano-grooved heat pipes. Int. J. Heat and Mass Tran., 132:280–287, 2019.

[6] D. Čoso, V. Srinivasan, M. C. Lu, J. Y. Chang, and A. Majumdar. Enhanced heat transfer
in biporous wicks in the thin liquid film evaporation and boiling regimes. J. Heat Transf., 134(10), 2012.

[7] Y. Nam, S. Sharratt, C. Byon, S. J. Kim, and Y. S. Ju. Fabrication and characterization of the capillary performance of superhydrophilic cu micropost arrays. J. Microelectromech. Syst., 19:581–588, 07 2010.

[8] R. Xiao, R. Enright, and E. N. Wang. Prediction and optimization of liquid propagation in micropillar arrays. Langmuir, 26:15070–5, 10 2010.

[9] R. Ranjan, A. Patel, S. V. Garimella, and J. Y. Murthy. Wicking and thermal characteristics of micropillared structures for use in passive heat spreaders. Int. J. Heat Mass Tran., 55(4):586–596, 2012.

[10] S. Ravi, D. Horner, and S. Moghaddam. Monoporous micropillar wick structures, i-mass transport characteristics. Appl. Therm. Eng., 73(1):1371–1377, 2014.

[11] Y. Zhu, D.S. Antao, Z. Lu, S. Somasundaram, T. Zhang, and E. N. Wang. Prediction and characterization of dry-out heat flux in micropillar wick structures. Langmuir, 32(7):1920–1927, 2016.

[12] G. Vaartstra, Z. Lu, and E. N. Wang. Simultaneous prediction of dryout heat flux and local temperature for thin film evaporation in micropillar wicks. Int. J. Heat Mass Tran., 136:170–177, 2019.

[13] J. E. Drummond and M. Tahir. Laminar viscous flow through regular arrays of parallel solid cylinders. Int. J. Multiph. Flow, 10:515–540, 1984.

[14] B. R. Gebart. Permeability of unidirectional reinforcements for rtm. J. Compos. Mater., 26(8):1100–1133, 1992.

[15] M. P. Sobera and C. R. Kleijn. Hydraulic permeability of ordered and disordered single-layer arrays of cylinders. Phys. Rev. E, 74:036301, 10 2006.

[16] A. Tamayol and M. Bahrami. Transverse permeability of fibrous porous media. Phys. Rev. E, 83:046314, 04 2011.

[17] K. Yazdchi, S. Srivastava, and S. Luding. Microstructural effects on the permeability of periodic fibrous porous media. Int. J. Multiph. Flow., 37(8):956–966, 2011.

[18] D. Horner, S. Ravi, and S. Moghaddam. Monoporous micropillar wick structures, ii-optimization & theoretical limits. Appl. Therm. Eng., 73(1):1378–1386, 2014.
[19] R. S. Hale, R. Ranjan, and C. H. Hidrovo. Capillary flow through rectangular micropillar arrays. Int. J. Heat Mass Tran., 75:710–717, 2014.

[20] R. S. Hale, R. T. Bonnecaze, and C. H. Hidrovo. Optimization of capillary flow through square micropillar arrays. Int. J. Multiphase Flow, 58:39–51, 2014.

[21] K. A. Brakke. The surface evolver. Exp. Math., 1(2):141–165, 1992.

[22] Y. Nam, S. Sharratt, G. Cha, and Y. S. Ju. Characterization and modeling of the heat transfer performance of nanostructured cu micropost wicks. J. Heat Transf., 133:101502, 10 2011.

[23] C. Byon and S. J. Kim. The effect of meniscus on the permeability of micro-post arrays. J. Micromech. Microeng., 21:115011, 10 2011.

[24] A. S. Sangani and A. Acrivos. Slow flow past periodic arrays of cylinders with application to heat transfer. Int. J. Multiph. Flow, 8(3):193–206, 1982.

[25] A. Tamayol and M. Bahrami. Analytical determination of viscous permeability of fibrous porous media. Int. J. Heat Mass Tran., 52(9):2407–2414, 2009.

[26] N. Srivastava, C. Din, A. Judson, N. C. MacDonald, and C. D. Meinhart. A unified scaling model for flow through a lattice of microfabricated posts. Lab on a chip, 10:1148–52, 05 2010.

[27] C. Zhang. Analytical and experimental investigation of capillary forces induced by nanopillars for thermal management applications. The Uni. of Texas at Austin, 05 2010.

[28] R. Ranjan, J. Y. Murthy, and S. V. Garimella. Analysis of the wicking and thin-film evaporation characteristics of microstructures. J. Heat Transf., 131:101001, 2009.

[29] R. Ranjan, J. Y. Murthy, and S. V. Garimella. A microscale model for thin-film evaporation in capillary wick structures. Int. J. Heat Mass Tran., 54(1):169–179, 2011.

[30] N. Farokhnia, P. Irajizad, S. M. Sajadi, and H. Ghasemi. Rational micro/nanostructuring for thin-film evaporation. J. Phys. Chem. C, 120:8742–8750, 2016.

[31] K. Montazeri, H. Lee, and Y. Won. Microscopic analysis of thin-film evaporation on spherical pore surfaces. Int. J. Heat Mass Tran., 122:59–68, 02 2018.

[32] M. Bongarala, H. Hu, J. Weibel, and S. V. Garimella. A figure of merit to characterize the efficacy of evaporation from porous microstructured surfaces. Int. J. Heat Mass Tran., 182:121964, 01 2022.
Micropillar wick evaporators with Marangoni convection

Yuncu et al.

[33] S. Adera, D. Antao, R. Raj, and E. N. Wang. Design of micropillar wicks for thin-film evaporation. Int. J. Heat Mass Tran., 101:280–294, 10 2016.

[34] R. W. Schrage. A Theoretical Study of Interphase Mass Transfer. Columbia University Press, New York, 1953.

[35] M. Wei, B. He, Q. Liang, S. Somasundaram, C. S. Tan, and E. N. Wang. Optimization and thermal characterization of uniform silicon micropillar based evaporators. Int. J. Heat Mass Tran., 127:51–60, 2018.

[36] S. Somasundaram, Y. Zhu, Z. Lu, S. Adera, H. Bin, W. Mengyao, S. T. Tan, and E. N. Wang. Thermal design optimization of evaporator micropillar wicks. Int. J. Therm. Sci., 134:179–187, 2018.

[37] H. Ghasemi and C. A. Ward. Energy transport by thermocapillary convection during sessile-water-droplet evaporation. Phys. Rev. Lett., 105(13):136102, 2010.

[38] Y. Kita, A. Askounis, M. Kohno, Y. Takata, J. Kim, and K. Sefiane. Induction of marangoni convection in pure water drops. Appl. Phys. Lett., 109(17):171602, 2016.

[39] O. Akdag, Y. Akkus, B. Cetin, and Z. Dursunkaya. Interplay of transport mechanisms during the evaporation of a pinned sessile water droplet. Phys. Rev. Fluids, 6:073605, 2021.

[40] J. R. Barber. The effect of thermal distortion on constriction resistance. Int. J. Heat Mass Tran., 14(6):751–766, 1971.

[41] V. P. Carey. Liquid-vapor Phase Change Phenomena. Hemisphere Publishing House, New York, 1992.

[42] COMSOL Multiphysics® v. 5.6. www.comsol.com. COMSOL AB, Stockholm, Sweden.

[43] Y. Akkus, A. T. Gurer, and K. Bellur. Drifting mass accommodation coefficients: in situ measurements from a steady state molecular dynamics setup. Nanosc. Microsc. Therm., 25(1):25–45, 2021.

[44] A. H. Persad and C. A. Ward. Expressions for the evaporation and condensation coefficients in the hertz-knudsen relation. Chem. Rev., 116(14):7727–7767, 2016.

[45] H. Hu and R. G. Larson. Analysis of the effects of marangoni stresses on the microflow in an evaporating sessile droplet. Langmuir, 21(9):3972–3980, 2005.
Declarations of interest

None.