Study of non-isothermal liquid evaporation in synthetic-micro-pore structures with hybrid LBM

Feifei Qin^{1,2,†}, Luca Del Carro³, Ali Mazloomi Moqaddam², Qinjun Kang⁴, Thomas Brunschwiler³, Dominique Derome² and Jan Carmeliet¹

¹Chair of Building Physics, Department of Mechanical and Process Engineering, ETH Zürich (Swiss Federal Institute of Technology in Zürich), Zürich 8093, Switzerland

²Laboratory of Multiscale Studies in Building Physics, Empa (Swiss Federal Laboratories for Materials Science and Technology), Dübendorf 8600, Switzerland

³Smart System Integration, IBM Research – Zurich, Saumerstrasse 4, 8803 Rüschlikon, Switzerland

⁴Earth and Environment Sciences Division (EES-16), Los Alamos National Laboratory (LANL), Los Alamos, NM 87545, USA

(Received xx; revised xx; accepted xx)

The mechanisms of non-isothermal liquid evaporation in micro-pore structures are studied both experimentally, and numerically by the lattice Boltzmann method. A hybrid thermal entropic multiple-relaxation-time multiphase lattice Boltzmann model (T-EMRT-MP LBM) is implemented and validated with experiments of droplet evaporation on a heated hydrophobic substrate. Then liquid evaporation is investigated in two specific pore structures i.e. spiral-shaped and gradient-shaped micro-pillar cavities, referred to as SMS and GMS. In SMS, the liquid receding front follows the spiral pattern; while in GMS, the receding front moves layer by layer from the pillar rows with large pitch to the rows with small one. Both simulations agree well with experiments. Moreover, evaporative cooling effects in liquid and vapor are observed and explained with simulation results. Quantitatively, in both SMS and GMS, the change of liquid mass with time coincides with experimental measurements. The evaporation rate generally decreases slightly with time mainly because of the reduction of liquid-vapor interface. Isolated liquid films in SMS increase the evaporation rate temporarily resulting in local peaks in evaporation rate. Reynolds and capillary numbers show that the liquid internal flow is laminar and that the capillary forces are dominant resulting in menisci pinned to the pillars. Similar Peclet number was found in simulations and experiments, indicating a diffusive type of heat, liquid and vapor transport. Our numerical and experimental studies indicate a method to control liquid evaporation paths in micro-pore structures and maintain high-evaporation rate by specific geometry designs.

Key words:

† Email address for correspondence: fqin@ethz.ch; feifei.qin@empa.ch

1. Introduction

Evaporative drying is a phenomenon present in many scientific and engineering processes, for example, design of new materials and structures, food preserving, and production of ceramics and paper. Recently, the self-assembly of nanoparticles induced by controlled evaporation of colloidal suspensions has attracted a lot of attention as a method for the fabrication of complex materials (Brunschwiler *et al.* 2016; Hamon *et al.* 2012; Boles *et al.* 2016). Zurcher *et al.* (2016) and Städler *et al.* (2017) have been working on nanoparticle self-assembly by non-isothermal evaporation to create underfills with high thermal conductivity applied as materials for electronic packaging. Hamon *et al.* (2012) conducted drying experiments of gold-nanorod-based materials on a textured substrate and observed that the self-assembled nanostructures are locally ordered as a smectic B phase, which could be used for amplifying optical signals. Boles *et al.* (2016) described that, different shapes of nanocrystal like spheres, polyhedral rods, can be used to design new functional materials with unique optical, magnetic, electronic and catalytic properties. In these studies, the self-assembly of nanomaterials is highly dependent on the control of drying of colloidal suspension. The drying pattern determines how and where the particles accumulate and assemble, while drying rate affects the yield of generation of self-assembled structures. Therefore, it is very essential to study the mechanisms of liquid drying in these micro-pore structures to guide the self-assembling processes.

Drying of pore structures includes heat and mass transfer problem that involves phase change, liquid and gas flows inside the porous medium, and diffusive or convective flows to the outside surrounding environment. The evaporation pattern and rate depend on the geometry of the structure as the pore size and distribution, and on the environmental conditions as the temperature, vapor pressure and air speed. Experiments have been done to study drying in micro-pore structures. Laurindo & Prat (1998) investigated the drying rate in a two-dimensional quasi-isothermal etched micromodel of three basic cases, namely without/stabilizing/destabilizing gravity, and found that thin liquid films have significant contributions to the drying rate. Yiotis *et al.* (2004) studied the effect of liquid films on the drying of porous media, and they found the effect to be dominant when capillarity controls the process. Pillai *et al.* (2009) studied slow evaporation of liquids in two-dimensional porous media with three sides insulated and one side exposed to air for drying. The porous medium was divided into two layers with different porosities and pores sizes, and only one layer was exposed to air. When larger-pore layer was exposed, the inner smaller-pore layer started drying only after the outer larger-pore layer was totally dried out, and the evaporation rate decayed. When smaller-pore layer was exposed, both the smaller-pore layer (due to evaporation) and larger-pore layer (due to capillary pumping) dried out and the evaporation rate was bilinear. Most recently, Chen *et al.* (2017, 2018) studied how to control drying kinetics by designing three different pore size distributions in micro-sized porous media. They demonstrated two types of control, i.e. the controlling the sequence of primary invasions through pore space and controlling the secondary liquid structures as films/bridges. For the liquid films/bridges, they provide hydraulic connectivity between the bulk liquid cluster and external rim. The bulk transports liquid to the rim due to capillary pumping, and the liquid at rims dry faster than at center since it is closer to open air. Therefore, a higher average evaporation rate was obtained. Fantinel *et al.* (2017) studied small-scale heterogeneity of the evaporation in micro-model made of pillar arrays, and observed no clear effect on how evaporation rates evolved. Besides the effects of external force, pore size/distributions and liquid films, the influence of temperature on drying patterns and drying rate was

explored. Vorhauer *et al.* (2013) compared isothermal and non-isothermal drying in a two-dimensional square pore network. These experiments showed that a stabilized gas-liquid region was established with decreasing temperature, while faster breakthrough and an extended two-phase zone were observed under isothermal condition. Vorhauer *et al.* (2011) also observed that drying patterns and drying rates are significantly depending on the direction of temperature gradient and pore size distribution.

The development of numerical models enables to simulate the drying processes, but taking into account accurately all drying phenomena remains a challenge. To describe the drying process, there are mainly two categories of numerical models: the continuum models and the pore network models. In continuum models, overall parameters like porosity, permeability and diffusivity are used to represent the transport properties of pore structures. Continuum models (Defraeye 2014) have been successfully used to study drying behavior in pore structures as fruits (Defraeye *et al.* 2013), porous plate (Defraeye *et al.* 2012). The continuum models are very efficient in computation, but they lack the ability to analyze local pore-scale drying phenomena. Pore network model (PNM), originally proposed by Fatt (1956), represents a porous medium as pores and throats, which interact according to different physical mechanisms such as capillarity, gravity, pressure dissipation by flow. Over the years, PNM has been improved by incorporating film effect (Prat 2007; Vorhauer *et al.* 2015), viscous effect (Metzger & Tsotsas 2008). The influence of temperature (Surasani *et al.* 2008, 2009) is also developed to simulate non-isothermal drying in two-dimensional (Taslimi Taleghani & Dadvar 2014) and three-dimensional (Surasani *et al.* 2010) pore networks. Through these developments, PNMs have become powerful tools to study drying of pore structures. However, PNMs remain approximations when simulating real complex porous material where pores and throats are not regular, or when the sizes of pores and throats are quite similar, even if based on actual X-ray CT (Blunt *et al.* 2013). The coupling of inner pore-scale liquid capillary flow as well as evaporation, with outside lab-scale vapor diffusion as well as gas convection remains complex in PNMs (Yiotis *et al.* 2007; Shaeri *et al.* 2013).

In last few decades, the lattice Boltzmann (LB) method has been widely used to study complex single phase and multiphase fluid flow in real complex pore structures (Kang *et al.* 2002; Boek & Venturoli 2010; Sukop & Or 2003; Huang *et al.* 2009; Chen *et al.* 2012, 2014; Liu *et al.* 2015, 2016; Li *et al.* 2016a). Because of the simplicity in dealing with complex wall boundary, LB models have proved to be very advantageous in simulating flow in pore structures. For simulating multiphase flow, LB models can capture the interface automatically by incorporating intermolecular-level interactions of kinetic nature, a feature which is very advantageous over traditional computational fluid dynamics (CFD) methods such as volume of fluid (Hirt & Nichols 1981) or level-set method (Sussman *et al.* 1994; Osher & Fedkiw 2001) that both require interface tracking and reconstruction. With the advantages of easily dealing with complex wall boundary and capturing interfaces automatically, LB models have already been successfully applied to study immiscible fluid flow in pore structures with effects of viscosity ratio, capillary number, wettability and gravity, under different permeability (Li *et al.* 2005; Ghassemi & Pak 2011; Huang *et al.* 2009). The above applications of LB models are all under isothermal conditions, while non-isothermal LB models are still under development and their applications are very limited. Recently, thermal multiphase LB models have been used to simulate non-isothermal droplet evaporation (Li *et al.* 2016b) and boiling (Li *et al.* 2015; Gong *et al.* 2018). Yu *et al.* (2017) have studied droplet evaporation on different heated heterogeneous solid surfaces. Zhang *et al.* (2015) simulated liquid thin film evaporation on a heated microstructural surface, and studied the heat transfer with

different surface wettability. However, the mechanisms of bulk liquid evaporation in pore structures are yet to be studied with LB models.

In the work described above, either the experiments lacked numerical validations, or the numerical models were still rough. In this paper, we study both numerically and experimentally non-isothermal bulk liquid evaporation in specifically designed micro pore structures, i.e. Spiral-shaped micro-pore structure (SMS) and Gradient-shaped micro-pore structure (GMS). Our proposed LB model here is more accurate in capturing the physics, and it helps us to understand the mechanisms better. Firstly, we introduce the T-EMRT-MP LBM and validate it with experiments in literature by simulating single droplet evaporation on a heated hydrophobic substrate. Then we briefly describe the experiments as well as the simulation setups. Finally liquid evaporation in SMS and GMS is simulated and compared with our experiment results both qualitatively and quantitatively. A better understanding of the evaporation process is obtained by investigating liquid mass, evaporation rate, liquid-vapor interface area and simulated heat transfer during evaporation. Results from our studies indicate ways to control liquid evaporation paths in pore structures as well as ways to maintain a high evaporation rate.

2. Model development

2.1. EMRT-MP LBM

We apply the EMRT-MP LBM to simulate two-phase flow. EMRT-MP LBM is developed by Qin *et al.* (2018) to simulate two-phase flow with a large range of Reynolds and Weber numbers at high density ratios. Here we briefly summarize the method. The LB equation for the populations of discrete velocities that incorporates the external force term is written as:

$$f_i(\mathbf{x} + \mathbf{v}_i, t + 1) = f'_i \equiv (1 - \beta) f_i(\mathbf{x}, t) + \beta f_i^{mirr}(\mathbf{x}, t) + F_i \quad (2.1)$$

The equilibrium populations f_i^{eq} maximize the entropy $S[f] = -\sum_{i=1}^Q f_i \ln(f_i/W_i)$ under fixed density and momentum $\{\rho, \rho \mathbf{u}\} = \sum_{i=1}^Q \{1, \mathbf{v}_i\} f_i^{eq}$, where W_i are the lattice weights (Karlin *et al.* 1999; Chikatamarla *et al.* 2006). The parameter $0 < \beta < 1$ is determined by the kinematic viscosity ν through $\nu = c_s^2(1/(2\beta) - 1/2)\delta t$. Here $c_s = \delta x/(\sqrt{3}\delta t)$ is the lattice speed of sound, and lattice units $\delta x = \delta t = 1$ are used with lattice speed $c = 1$. The mirror state is constructed at each lattice site and every time step from the entropy maximization of the summarized post-collision population f'_i by relaxing high order moments properly (Karlin *et al.* 2014; Bösch *et al.* 2015).

The last term $F_i = [f_i^{eq}(\rho, \mathbf{u} + \Delta \mathbf{u}) - f_i^{eq}(\rho, \mathbf{u})]$ in Eq. 2.1 represents the fluid-fluid cohesive force for phase separation and the fluid-solid interaction for realizing various wettability. The forces are implemented by evaluation of the flow velocity increment $\Delta \mathbf{u} = \mathbf{F}\delta t/\rho$ with the force $\mathbf{F} = \mathbf{F}_c + \mathbf{F}_w$. Real velocity of the fluid including the force term is $\mathbf{u}_f = \mathbf{u} + \Delta \mathbf{u}/2$. To obtain a tunable surface tension, the multirange pseudopotential-based cohesive force is applied as (Sbragaglia *et al.* 2007):

$$\mathbf{F}_c = -\psi(\mathbf{x}) \sum_{i=1}^Q w(|\mathbf{v}_i|^2) [G_1 \psi(\mathbf{x} + \mathbf{v}_i) + G_2 \psi(\mathbf{x} + 2\mathbf{v}_i)] \mathbf{v}_i \quad (2.2)$$

where the interaction potential $\psi = \sqrt{2(P_{EoS} - \rho c_s^2)/[(G_1 + 2G_2)c^2]}$, and G_1, G_2 are coefficients to tune the surface tension. P_{EoS} is the equation of state (EoS), and here we adopt the Carnahan-Starling (C-S) EoS (Yuan & Schaefer 2006). The other force

fluid-solid interaction, is represented as:

$$\mathbf{F}_w = -\psi(\mathbf{x}) \sum_{i=1}^Q w(|\mathbf{v}_i|^2) [G_1 \psi(\rho_w) I(\mathbf{x} + \mathbf{v}_i) + G_2 \psi(\rho_w) I(\mathbf{x} + 2\mathbf{v}_i)] \mathbf{v}_i \quad (2.3)$$

where I is the indicator function that equals unity at solid nodes and zero at fluid nodes, and ρ_w the parameter to determine wettability. $w(|\mathbf{v}_i|^2)$ in $\mathbf{F}_c$ and $\mathbf{F}_w$ are appropriately chosen weights (Yuan & Schaefer 2006). With this EMRT-MP LBM, two-phase flow can be simulated for a large range of fluid viscosity and tunable surface tension (Qin *et al.* 2018).

2.2. T-EMRT-MP LBM

To model non-isothermal evaporation, the equation for heat transport in liquid and vapor phases including latent heat is coupled to the EMRT-MP LBM, referred to as T-EMRT-MP LBM. The heat transport equation is derived from the local balance law for entropy (Anderson *et al.* 1998). By neglecting viscous heat dissipation, the governing equation for temperature (T) transport can be written as (Li *et al.* 2016b; Yu *et al.* 2017):

$$\partial_t T = -\mathbf{u}_f \cdot \nabla T + \frac{1}{\rho C_V} \nabla \cdot (\lambda \nabla T) - \frac{T}{\rho C_V} \left(\frac{\partial P_{EOS}}{\partial T} \right)_P \nabla \cdot \mathbf{u}_f \quad (2.4)$$

where ρ is the fluid density, λ is the thermal conductivity and C_V is the specific heat at constant volume. The first two terms on the right hand side of Eq. 2.4 represent heat convection and conduction respectively, while the last term corresponds to the latent heat for phase change. There are two approaches to solve the extended temperature equation. The first method is to use an-other lattice Boltzmann equation with a source term, which induces error terms in the recovered macroscopic temperature equation, as explained by Li *et al.* (2017). The recently developed Gong model (Gong *et al.* 2018) uses this method. The other way is to solve it with traditional numerical schemes like finite difference method (FDM). In this way, no error terms are introduced and the model is more accurate. In our paper, this equation is solved by FDM with second-order Runge-Kutta scheme for time discretization:

$$T^{t+\delta t} = T^t + \frac{\delta t}{2} (h_1 + h_2) \quad (2.5)$$

where h_1, h_2 are given as

$$h_1 = F(T^t), h_2 = F(T^t + \delta t * h_1) \quad (2.6)$$

and $F(T)$ represents the right-hand side of Eq. 2.4 while δt is the time step in numerical iteration. For spatial discretization, isotropic central schemes are employed to evaluate the first-order derivative and the Laplacian (Lee & Lin 2005).

The two-way coupling between EMRT-MP LBM and temperature equation works as this: at each time step, flow variables like density, velocity and pressure are firstly computed by solving EMRT-MP LBM; then they are plugged into temperature equation to update temperature field; finally the updated temperature is incorporated in computing flow field by equation of state for the next time step. The mesh used for solving temperature equation is the lattice in EMRT-MP LBM, and in this way extra interpolations are not necessary for data exchange. The detailed explanation of how evaporation is shown in Appendix A.

2.3. Validation of T-EMRT-MP LBM

The study of droplet evaporation has been of intensive interest both in experimental and numerical research (Dunn *et al.* 2009; Stauber *et al.* 2014; Saxton *et al.* 2016). For a droplet of diameter D evaporating at a constant temperature, the evaporation process is described by the well-known D^2 law. The law shows that the square of the droplet diameter decreases linearly with evaporation time, i.e. $D^2(t)/D_0^2 = 1 - K * t$, and that the coefficient K is linearly dependent on thermal conductivity λ (Law 1982). Dash & Garimella (2013) studied experimentally droplet evaporating on hydrophobic and superhydrophobic surfaces, and their results were shown to follow the D^2 law. Our model is a non-isothermal model, but it can be used to simulate this quasi-isothermal drying case by certain simulation setups. In Appendix A, we have simulated a single droplet evaporation in a closed cavity and compared with the diameter square law as well as the result from Gong *et al.* (2018), to show the accuracy of our model. Since we mainly study the non-isothermal evaporation in the paper, we validate our T-EMRT-MP LBM with droplet evaporation on a heated hydrophobic surface by comparing the evolutions of droplet volume, radius and contact angles with experiment results (Dash & Garimella 2014).

In the experiments by Dash & Garimella (2014), the droplet is gently deposited on a heated surface with different temperatures. The droplet size is small, i.e. $3 \pm 0.1 \mu L$ so that the gravity can be neglected. The experiments are done in ambient conditions with an air temperature of $T_{air} = (21 \pm 0.5)^\circ C$ and relative humidity $(36 \pm 2)\%$. We consider two experiments with different surface temperatures of $40^\circ C$ and $50^\circ C$. The surface has a contact angle of 120° initially when the experiments start. The evaporation happens in a relative static ambient condition without air flow, thus the convective evaporation is neglected and diffusive evaporation is considered. Our simulations are carried out in a three-dimensional domain with $N_x \times N_y \times N_z = 160 \times 160 \times 100$ lattices³, with a droplet of diameter of $D_0 = 70$ lattice nodes initially located in the center of a heated substrate. The lateral four sides and top boundary conditions are zero gradient for both velocity and temperature. The zero gradient velocity boundary allows vapor flowing out freely. The density ratio of liquid and vapor is $\rho_l/\rho_v \approx 30$ with temperature ratio at $T/T_c = 0.75$, where T_c is the critical temperature. The vapor temperature is set as saturation temperature $T_{vapor} = T_{sat} = 0.75T_c$ while the substrate surface is considered to be a non-slip wall at a temperature of $T_{w1} = 0.778T_c$ and $T_{w2} = 0.794T_c$ for the cases of $40^\circ C$ and $50^\circ C$ surface temperature. These non-dimensional temperatures are chosen to keep the relative temperature differences in simulations similar as in the experiments, i.e. $(T_{w1} - T_{vapor})/T_c = 2.8\% \approx (40 - 21.5)/647 = 2.85\%$ and $(T_{w2} - T_{vapor})/T_c = 4.4\% \approx (50 - 21.5)/647 = 4.41\%$, where $T_c = 647K$ is the water critical temperature. As $T_w > T_{vapor}$, the droplet gradually evaporates because of the heat conducted from the substrate to the boundaries. The evaporation continues because of the difference in vapor pressure between the liquid-vapor interface and outlet as explained in section 2.2. Note that all the variables here are in lattice units, and the analysis in the following work is based on the similarity of non-dimensional numbers between experiment and LBM, as discussed below, guaranteeing similar fluids and heat/mass transport phenomena being studied in experiment and LBM.

The analysis of droplet evaporation is analyzed using normalized variables, i.e. $V_N = V(t)/V_0$, $r_N = r(t)/r_0$ and $t^* = t/t_0(T_{w1})$, where V_0 , r_0 and $t_0(T_{w1})$ are the initial droplet volume, contact radius and total evaporation time at a substrate temperature of T_{w1} . Using $t_0(T_{w1} = 0.778T_c)$ as a reference, we can compare the different evaporation

Figure 1: Evaporating droplet at normalized time $t^*=0.14$. a) half-droplet cross-section profile and boundary conditions; b) temperature contours; c) streamlines inside (Marangoni flow) and outside droplet (evaporated vapor)

Figure 2: Comparisons between T-EMRT-MP LBM simulations and experiments. a) normalized droplet volume; b) normalized droplet contact radius; c) droplet contact angle

rates for the different temperature cases, i.e. $T_{w1} = 0.778T_c$ and $T_{w2} = 0.794T_c$. Figure 1 shows the results for an evaporating droplet on a heated substrate with temperature $T_{w1} = 0.778T_c$ at normalized time $t^*=0.14$. In figure 1b we show the temperature distribution in and outside the droplet. We observe that the temperature decreases from the substrate to the outside. Because of the temperature variation at the liquid-vapor interface, the surface tension changes. Higher surface tension appears at locations of lower temperature introducing a surface flow from bottom to top on the surface of the droplet. This surface flow induces a vortex flow inside the droplet, known as Marangoni flow (Li *et al.* 2016b; Liu *et al.* 2013, 2014; Wodlei *et al.* 2018). In figure 1c, we show the Marangoni flow, which qualitatively validates our model.

In figure 2 we compare quantitatively the time evolution of normalized volume, contact radius as well as contact angle for experiment and simulation. Overall, we observe a good agreement between our simulation results and experiments, both showing a decrease of droplet volume and contact radius with time. In the experiments, the total evaporation time for a plate temperature of $50^\circ C$ is around 55% of that for a temperature of $40^\circ C$, which is also captured by the simulations. The variation in contact angle in the simulations is smaller compared with the experiments. Possible reason is that the heated surface is assumed to be totally smooth in the simulations, while in experiment it is not.

Figure 3: Schematic representation of micro-pore structure: a) side view; b) top view.

Figure 4: Top view of the experimental area of a) spiral-shaped micro-pore structure (SMS) and b) gradient-shaped micro-pore structure (GMS). The height of SMS and GMS is $60 \mu m$.

According to Dash & Garimella (2014), the roughness of surface may lead to a 10° contact angle hysteresis. By the end of the evaporation process, the change in contact angle in experiment becomes more obvious, with values below 40° while in the simulations, the decrease is less. However, in general, our T-EMRT-MP LBM simulation results agree well with the experimental results both qualitatively and quantitatively.

3. Experiment setups and procedures

In this paper, the liquid evaporation was studied in micro-cavities containing arrays of squared-Silicon (Si) micro-pillars, which were fabricated by photolithography and reactive-ion etching, obtaining a pillar height of $60 \mu m$ (figure 3a). These pillars were aligned in spiral-shaped (SMS) and gradient-shaped (GMS) geometries, respectively. In typical porous media, there are two main drying periods, i.e. the constant rate period

Figure 5: Experimental setup for liquid evaporation in micro-pore structure: a) schematic representation; b) photo of experimental setup with zoom of micro-pore structure

(CRP) and the decreasing rate period (DRP) (Yiotis *et al.* 2006; Irawan 2006). The CRP is due to the capillary pumping effect, which is the liquid internal transport from large pore spaces inside the porous media to small ones at vaporization plane. The DRP is when the pores filled with liquid are around same size, and the pumping effect is very weak. The CRP is usually shorter compared to DRP, which makes the average drying rate small. The geometries of SMS and GMS are designed with certain pore spaces to trigger the onset of capillary pumping, and to keep it until the end of drying. In this way, the liquid evaporation path follows the specific designs, and the liquid evaporation rate is increased, compared to typical porous media. The evolution of evaporation rate in SMS and GMS are shown in Section 5.1 and 5.2, respectively. SMS is designed with two different values $180\ \mu\text{m}$ and $80\ \mu\text{m}$ for the distance between the pillars (figure 4a), while in the GMS the pillar distance gradually decreases layer by layer (figure 4b). Subsequently, a glass lid was bonded on top of the pillars to form the micro-pore structure, allowing visual inspection during the evaporation process. Before the experiments, the cavities were treated with oxygen plasma for 5 minutes at 600W (PVA TePla GIGAbatch 310 M) in order to get a uniform contact angle on the surfaces. After this treatment, the measured contact angle varies between 35° and 39° . To avoid the influence of liquid remaining stuck at the edges of the plates, a fence of pillars was placed around the experimental area, and is referred as “protection pillars” (figure 3b) in the following text. The distance D (in green) is chosen as the characteristic length for liquid flow. The red dash-dot arrows indicate the expected flow direction. L is the total length that a liquid meniscus travels during the evaporation process. In SMS, L is the total length of spiral shape, while in GMS, $L = 7L_0$, is the sum of the half-length of each layer. These dimensions are used to determine non-dimensional numbers as shown below.

For the experiment, the micro-pore structure was placed on a hot plate fixed at a constant temperature of 50°C (figure 5a). A solution of DI water and fluorescein was injected in the micro-cavity and the fluorescence was excited by a lateral illumination source ($455 < \lambda < 495\ \text{nm}$) and filtered by an emission filter ($500 < \lambda < 550\ \text{nm}$) before being collected by a camera (ace acA2040-90, Besler). Images were recorded every 1 s during the entire evaporation of the solution (figure 5b). After the experiment, the recorded images were processed with ImageJ (Stalder *et al.* 2010) to extract information for detailed analysis seen in section 5.

4. Simulation setups

Given the small height to length ratio (6/500) of the micro-pore structure, we first simulate the evaporation process in two dimensions (2D). A comparison with a three-dimensional (3D) simulation is provided in section 6. In the experiment the temperature is kept constant at 50°C by heating the hot plate. Since the thermal conductivity of silicon is high ($130\text{ W}/(\text{mK})$), it is reasonable to assume that the silicon plate and pillars are at the same temperature as the aluminum plate. This assumption of equal temperature in plate and pillars is supported by measurements of the temperature difference across the cavity from the bottom of silicon to the top of the glass plate, which was found to be less than 1°C . It is important to note that in 2D the heated silicon pillars are the only heat sources, while in 3D the plate is also a heat source. We simulated the evaporation process for different liquid-vapor density ratios ranging from 15 to 60 and found that the results are not sensitive to this ratio. To save computational time while maintaining a sufficiently high value for the surface tension, the density ratio of liquid over vapor is chosen to be $\rho_l/\rho_v \approx 30$ with a vapor temperature equal to the saturation temperature $T_{\text{vapor}} = T_{\text{sat}} = 0.75T_c$ and a pillar temperature $T_{pl} = 0.76T_c$. The pillar temperature is set to make sure all the mechanisms during drying are the same as in the experiments (see section 5 and Appendix D). The temperature boundary conditions at the four lateral sides are assumed to be Neumann boundary conditions, with a temperature gradient equal to zero. The boundary condition for vapor flow is a zero gradient velocity condition at the four lateral sides so that vapor can flow out freely. Heat at the boundary is thus transported out of the computational domain convectively by vapor transport. The size of pillars is $7 \times 7 \text{ lattices}^2$ and the pillars are located similarly as in the experiments. In our LBM simulations, the liquid-vapor interface is a smooth boundary over 4 to 5 lattices. The pillar size is sufficiently larger than the interface thickness so that interface effects can be neglected, meaning pinning of the interface will occur at the pillars edges.

In the area of fluid mechanics, dimensionless parameters allow us to analyze simulation and experimental results, as they often control the behavior of a physical system. In our case, the relevant dimensionless control parameters determine the evaporation patterns. In this paper, the Reynolds, capillary and Peclet numbers are used to evaluate the similarity between our simulations and experiments. For fluid flow, the Reynolds and capillary numbers are used. The Reynolds number $Re = \overline{u_m}D/v$ is defined as the ratio of inertial to viscous force, while the capillary number $Ca = \rho_l v \overline{u_m} / \sigma$ is the ratio of viscous to capillary force, where ρ_l , v and σ are liquid density, kinematic viscosity and surface tension. For heat and mass transport, we also use the Peclet number $Pe = \overline{u_m}D/D_v$, which is the ratio of convective and diffusive transport of heat or mass and D_v represents the thermal or mass diffusivity. The fluid properties such as thermal conductivity, heat capacity and viscosity are set according to the values in the experiments. D is a characteristic length taken as the distance between pillars in the center of the evaporation path (see figure 4). D is equal to $180\text{ }\mu\text{m}$ (63 lattices) for SMS and $115\text{ }\mu\text{m}$ (38 lattices) for GMS. $\overline{u_m}$ is the average velocity of the main liquid meniscus. In SMS, the average velocity of the main liquid meniscus is defined as $\overline{u_m} = L/t_{\text{tot}}$, where L is the total distance travelled by the evaporation front (length of red line in figure 4a) and t_{tot} is the total evaporation time. In GMS, the evaporation front travels layer by layer from large pore rows to small ones resulting in $L = 7L_0$.

5. Two-dimensional results and discussion

5.1. Liquid evaporation in spiral-shaped micro-pore structure (SMS)

We first analyze the liquid configurations during the evaporation process in SMS. Different frames are compared in figure 6a-b for experiment (supplementary movie 1) and simulation (supplementary movie 2). The evaporation process follows a spiral route as we designed. A good agreement between experiment and simulation results is observed. To understand the origin of this spiral pathway, we analyze the density, liquid pressure distribution and velocity contour at time $t = 32.87s$ (figure 7). We observe in figure 7b that the liquid pressure is higher at the major meniscus showing a large radius of curvature, while the liquid pressure is lower at the minor menisci, showing smaller radii of curvature. According to Laplace law, the capillary pressure scales with the surface tension σ divided by the radius of curvature of the meniscus r , or $P_\sigma \propto \sigma/r$. If we neglect temperature difference at different menisci, the surface tension σ can be assumed the same at all menisci. This means that the capillary pressure P_σ at the major meniscus is lower than that at the minor menisci. Assuming the vapor pressure is constant in the vapor phase and in equilibrium with the liquid pressure at the menisci, the liquid pressure is then given by $P_l = P_v - P_\sigma$. This means that the liquid pressure will be higher at the major meniscus than at the minor menisci, as is found in our simulations. This pressure difference leads to an internal liquid flow from major to the minor menisci as also shown in the velocity contours in figure 7c. This shows that evaporation mainly happens at the minor menisci, while the movement of the major meniscus results from the internal liquid flow driven by the liquid pressure difference.

Figure 6c shows the temperature distribution (supplementary movie 3) during the evaporation process. The temperature drops at the menisci due to evaporative cooling. The vapor phase is cooled down in a zone around the evaporating menisci (zone in blue color in figure 6c). The vapor phase remains colder at the consecutive times $t = 85.19, 112.10, 136.00$ except at zones around the pillars, where the vapor is locally heated up by the hot pillars. In the liquid phase, heat is transported from the heated pillars immersed in the liquid phase. A temperature gradient is observed from inside the liquid to the evaporating menisci. **The average and maximum temperature variations in the 2D simulation are shown in figure 8d. We can see that the average and maximum temperature drops are around 2.66 K and 10.0 K.** Next, by studying the Peclet number for heat flow in liquid and vapor phase, we analyze whether the heat transport is diffusive (conduction) or convective (by fluid flow). It is worth mentioning that the temperature difference in the 2D simulation is found to be larger than that in 3D results, which is presented below.

Figure 8a shows the evolution of liquid mass m with time t for the experiment and simulation. A good agreement between simulation and experimental results is observed. Figure 8b gives the evaporation rate Ep versus time. The evaporation rate gradually decreases with time showing some temporary peaks. Figure 8c gives the liquid-vapor interface I versus time. The global decrease in evaporation rate is closely related to the decrease in interfacial area as shown in figure 8e-f, for simulation and experiment respectively. The local peaks correspond to temporary higher evaporation rates when the major meniscus passes a corner of the spiral path (figure 8e-f). Liquid configurations at two selected peaks for both simulation ($t = 28.33s$ and $t = 77.87s$) and experiment ($t = 20.98s$ and $t = 72.81s$) are illustrated in figure 8g. After passing the corner, the major meniscus breaks up leaving an isolated liquid island within the corner pillars.

Figure 6: Different frames of liquid evaporation in SMS. a) liquid distribution from experiment (supplementary movie 1); b) and c) density (supplementary movie 2) and temperature distribution (supplementary movie 3) from 2D T-EMRT-MP LBM simulation. Density (ρ) and temperature (T) are in lattice units while time (t) is in physical unit [s].

Figure 7: Explanation of spiral route with a) density, b) pressure and c) velocity contour at physical time $t = 32.87s$. Density (ρ) pressure (p) and velocity ($velo$) are in lattice units.

These liquid islands evaporate faster compared to bulk liquid due to their high perimeter to area ratio, accounting for the peaks in evaporation rate.

The evaporation rates of the 2D simulation and experiment follow the same trend until about $t \approx 116s$, after which the evaporation rate keeps relatively constant in the experiment, while it continuous to decrease in the simulation. This observation may be explained by the fact that, in the 2D simulation, the heat comes only from the heated pillars, while, in the experiment, both pillars and base silicon plate are heated. Therefore, the thermal energy available for evaporating the liquid is less in the 2D simulation with respect to the experiment. This lower thermal energy slows down the evaporation rate

Figure 8: Analyses of liquid evaporation in SMS. a), b) comparison of liquid mass, evaporation rate between experiment and simulation; c) comparison of liquid-vapor interface area between experiment and simulation; d) average and maximum temperature variation in simulation; e) and f) comparison of evaporation rate and liquid-vapor interface in simulation and experiment; g) comparison of liquid film between pillars after the main meniscus passes the corner between simulation (at $t = 28.33s$ and $t = 77.87s$) and experiment (at $t = 20.98s$ and $t = 72.81s$). All variables are in physical units.

in simulation compared to experiment. Additionally, the higher evaporation rate in the experiment at the end of the evaporation process ($t = 136.00s$) can be attributed to the evaporation of a film tail of liquid (figure 6a), which does not appear much in the simulation (figure 6b). In section 6, we show that we can improve the simulation results when simulating the evaporation process in 3D taking into account heat also provided from the silicon plate. In the experiment of drying in SMS, the ratio of the average evaporation rate over the maximum evaporation rate is $Ep_{aver}/Ep_{max} = 81.5\%$, which

	Re_L	Re_V	Ca	$Pe_{L,T}$	$Pe_{V,m}$
Exp.	0.014	0.006	3.51E-7	0.05	3.68E-3
2D LBM	1.740	0.420	2.33E-2	0.71	1.30E-3
mechanism	laminar flow	laminar flow	capillary force dominant	diffusion dominant	diffusion dominant

Table 1: Non-dimensional numbers for experiment and 2D LBM simulation in SMS

means the evaporation rate is generally constant. One main reason is the contribution of capillary pumping as explained in section 3, and the other one is the high energy supply with the heating temperature of $T_p = 50^\circ C$. The high temperature difference between the micro-pillar structure and the environment ($T = 22^\circ C$) speeds up the vapor diffusion process, which highly increases the evaporation rate. Thus, the SMS geometry as well as the heating source helps to maintain high evaporation rate during the entire drying process.

Now we evaluate the non-dimensional numbers as described in section 4. In the experiment, the temperature of the hot plate is at $50^\circ C$, at which the properties of water are $\rho_l = 988 \text{ kg/m}^3$, $v_L = 5.53E-7 \text{ m}^2/\text{s}$, $\sigma = 6.79E-2 \text{ N/m}$, respectively. The average velocity of the main evaporation meniscus is $\bar{u}_m = L/t_{tot} = 5.93E-3/136 = 4.36E-5 \text{ m/s}$. The dimensionless numbers for liquid phase then are a Reynolds number of $Re_L = 0.014$ and a capillary number of $Ca = 3.51E-7$. As the Reynolds number is small, the liquid internal flow is in the laminar regime. The capillary number is very small, which means the capillary forces are much more dominant than the viscous forces. For our 2D simulation in SMS, the iteration steps are 364,000 with 7.0 CPU hours of 64 processors, leading to the average velocity of main meniscus $4.61E-3$ lattice units. We calculated the corresponding non-dimensional numbers as $Re_L = 1.74$ and $Ca = 2.33E-2$. The Reynolds and capillary numbers in simulations are not as low as in the experiment, due to the limitation of the LB models, i.e., the velocity cannot be very low and surface tension cannot be very high (Yuan & Schaefer 2006; Qin et al. 2018). However, both numbers indicate that the simulated flow characteristics are in the similar regime as in the experiment, i.e. laminar flow and capillary forces dominating viscous forces, which accounts for the good agreement between experiments and simulations.

The Reynolds numbers for vapor flow in experiment and simulation are $Re_V = 5.57E-3$ and $Re_V = 0.42$, respectively. Therefore, the vapor flow is also in the laminar regime. Heat transport from the pillars to the liquid phase is found to be important since it mainly affects the energy supply controlling the evaporation. Therefore, we compare the Peclet number of heat transport in the liquid phase $Pe_{L,T}$ for simulation and experiment. We obtain $Pe_{L,T} = 0.05 < 1$ in the experiment and $Pe_{L,T} = 0.71 < 1$ in the simulation, which indicates that the heat transport in the liquid phase is dominated by diffusion rather than convection. For example at $t_N = 20.71$ in figure 6c, the liquid temperature distribution does not follow the internal liquid flow, indicating that the convective heat flow is rather negligible compared to heat diffusion. We further study the type of vapor transport in simulation and experiment. In experiment, the Peclet number of vapor mass transport is $Pe_{V,m} = Re_V * Sc_V = 3.86E-3$, with $Sc_V = v_V/D_V$ the Schmidt number, where $v_V = 2.08E-5 \text{ m}^2/\text{s}$ and $D_V = 3.0E-5 \text{ m}^2/\text{s}$ are the vapor kinematic viscosity and mass diffusivity at $50^\circ C$. In the simulation, the mass diffusivity is more difficult to

Figure 9: Analyses of liquid evaporation in SMS (2D). a) liquid configuration during evaporation with heated pillar temperature $T_{pl} = 0.80T_c$; b) and c) comparison of liquid mass and evaporation rate with $T_{pl} = 0.80T_c$ and $T_{pl} = 0.76T_c$. All variables are in physical units.

determine. We first estimate the average density gradient $\Delta\rho_V/\Delta L_V = (\rho_{V_2} - \rho_{V_1})/\Delta L_V$ from liquid-vapor interface to outlet, with ρ_{V_2} the vapor density at the interface and ρ_{V_1} the vapor density at the outlet boundary, and ΔL_V the average distance from interface to outlet. We also calculate the mass flux $q = \Delta m_L/(A_V * t)$ through evaporation, and finally obtain the vapor diffusivity as $D_V = q/(d\rho_V/dL_V)$. In our simulation, the kinematic viscosity of vapor is $\nu_V = 0.167$. Then we calculate the Peclet number as $Pe_{V,m} = Re_V * Sc_V = 1.30E - 3$, which is in the similar range as in experiment. This means that the vapor transport is diffusive. All the non-dimensional numbers discussed above are summarized in Table 1.

The capillary number Ca affects the capillary pumping effect, and the smaller the capillary number, the stronger the pumping. The evaporation pattern is determined by the competition between pumping effect and local evaporation rate (controlled by temperature gradient by liquid and environment). If the pumping effect is stronger than the local evaporation, the liquid remains pinned to the pillars, which is the cases in our experiment that we see the spiral pattern in SMS. Otherwise the drying pattern will be quite different. Since the heating temperature affects the liquid property like surface tension as well as the drying rate, changing temperature results in different evaporation patterns. For example, when we raise the heating temperature of pillars from $T_{pl} = 0.76T_c$ to $T_{pl} = 0.80T_c$, the capillary number Ca increases from $2.33E - 2$ to $1.40E - 1$, and the evaporation pattern changes form from “spiral” to “continuous” as shown in figure 9a. The liquid mass and evaporation rate shown in figure 9b and c of $T_{pl} = 0.80T_c$ also change dramatically, compared to those of $T_{pl} = 0.76T_c$. Therefore, the characteristic capillary number for the spiral pattern in SMS is between $2.33E - 2$ and $1.40E - 1$. With other non-dimensional numbers guaranteed in the similar range as experiment, any capillary number no more than $2.33E-2$ is small enough to simulate the same evaporation pattern as well as the evaporation rate.

Figure 10: Frames of liquid evaporation in GMS. a) liquid distribution from experiment (supplementary movie 4); b) and c): density (supplementary movie 5) and temperature contour (supplementary movie 6) from T-EMRT-MP LBM simulation. Density (ρ) and temperature (T) are in lattice units while time (t) is in physical unit [s].

Figure 11: Explanation of layer by layer evaporation route with a) density, b) pressure and c) velocity contour at physical time $t = 51.36s$. Density (ρ) pressure (p) and velocity ($velo$) are in lattice units.

5.2. Liquid evaporation in gradient-shaped micro-pore structure (GMS)

Figure 10 a and b show frames of different liquid configurations for the GMS case, for experiment (supplementary movie 4) and simulation (supplementary movie 5), respectively. Again a good agreement can be observed. The frames show that the liquid evaporation front moves mainly layer by layer from the top row with larger pillar distance to the lower rows with decreasing pillar distance. The larger distance between the pillars in the higher rows leads to menisci with larger radius of curvature, which according to Laplace law leads to lower capillary pressure or higher liquid pressure. The lower rows with smaller distance between the pillars result in lower liquid pressures. The pressure difference from large to small pore rows, as seen in figure 11b at $t = 51.36s$, leads to an

Figure 12: Analyses of liquid evaporation in GMS. Comparison of a) liquid mass, b) evaporation rate and c) liquid-vapor interface area between experiment and simulation; d) average and maximum temperature variation during drying; comparison of e) evaporation rate and f) liquid-vapor interface in simulation and experiment. All variables are in physical units.

internal liquid flow from large menisci to small ones (figure 11c). The liquid front thus moves downwards row by row until all liquid is evaporated from the smallest pore row. The temperature field (figure 10c, supplementary movie 6) shows evaporative cooling at the evaporating menisci: a cooled down vapor zone next to these menisci with locally heated zones due to the presence of hot pillars, and a hotter liquid zone heated by the pillars immersed in the liquid phase. The average and maximum temperature variations in the 2D simulation are shown in figure 12d. We can see that the average and maximum temperature drops are around 1.57 K and 4.6 K .

Figure 12a shows that the changes of liquid mass with time in the experiment and simulation are in good agreement. The evaporation rate (figure 12b) in both experiment and simulation fluctuates while decreasing with time. figure 12c gives the liquid-vapor interface I_N versus time. Figure 12e and f show the relations between evaporation rate and liquid-vapor interfacial area for simulation and experiment, respectively. We observe a close relation between the evaporation rate and interfacial area. The fluctuation behavior can be explained by the consecutive de-pinning of menisci in a row resulting in a local increase of the evaporation rate. At the end of the evaporation process after $t \approx 95\text{ s}$, the evaporation rate continuously decreases in the simulation while it increases again in the

	Re_L	Re_V	Ca	$Pe_{L,T}$	$Pe_{V,m}$
Exp.	0.006	0.015	2.25E-7	0.02	1.03E-3
2D LBM	0.570	1.240	1.44E-2	0.23	1.56E-3
mechanism	laminar flow	laminar flow	capillary force dominant	diffusion dominant	diffusion dominant

Table 2: Non-dimensional numbers for experiment and 2D LBM simulation in GMS

experiment. The reason is also attributed to the fact that less thermal energy available for evaporation in the simulation compared to the experiment as explained in section 5.1. In the experiment of drying in GMS, the ratio of the average evaporation rate over the maximum evaporation rate is $Ep_{aver}/Ep_{max} = 79.0\%$, indicating the evaporation rate is generally constant. Similar to SMS, the GMS geometry also helps to maintain high evaporation rate during the entire drying process with the heat source.

In GMS, the evaporation time in experiment is 107s, while the iteration steps in simulation is 300,000 (6.6 CPU hours with 64 processors). Similar to the SMS case, we have determined the non-dimensional numbers for both experiments and simulations in GMS, as shown in table 2. The range of non-dimensional number shows that the flow, heat and mass transport mechanisms are laminar, capillary driven, and diffusion dominated.

6. Three-dimensional results

In the 2D simulations presented above, heat is provided only by the pillars, while in the experiment, both the silicon plate and pillars serve as heat sources. Moreover, the menisci in the experiment have a more complex 3D shape, which cannot be captured in a 2D simulation. To verify the accuracy of a 2D simulation, we carried out a 3D simulation for SMS. The ratio of height to length/width is set identical to the one in experiment, and other dimensions remain the same as in the 2D simulation. The 3D simulation setup is shown in figure 13. The silicon plate and pillars are set to a temperature of $T_h = 0.751T_c$, which is slightly larger than the saturation temperature $T_s = 0.75T_c$. We used a lower surface temperature of the heat source in order to render the non-dimensional numbers in experiment and simulations comparable. The lower surface temperature in 3D compared to 2D can be explained by the fact that heat is more efficiently transported to the liquid in 3D with both the bottom silicon plate and pillars as heat sources. The top glass is set adiabatic, since the measured glass temperature was close enough to the surface temperature of the silicon plate. We impose zero velocity gradient (allowing free vapor outflow) at the four boundary sides, similar as in the 2D case. For the temperature at the four lateral sides T_l , to consider the heating up effect of bottom hot plate during drying, we assume T_l increases linearly with time until the drying completes when T_l becomes identical to T_h .

Different frames for the 3D simulation are shown in figure 14. The spiral evaporation route (supplementary movie 7) is the same as in the 2D simulation and experiment. The menisci have now a 3D shape as shown in figure 13. A more striking difference from the 2D simulation is much smaller zones cooled by evaporation in the temperature field

Figure 13: Illustration of 3D T-EMRT-LBM simulation setup of SMS with zoom of 3D menisci.

Figure 14: Frames of liquid evaporation in SMS from 3D T-EMRT-MP LBM simulation. a) liquid configuration (supplementary movie 7); b) temperature contour (supplementary movie 8) of cross-section. Temperature (T) is in lattice unit while time (t) is in physical unit [s].

(supplementary movie 8), and smaller temperature differences between vapor and liquid phase as shown in figure 14b. These are caused by the strong heating effect of the bottom silicon plate. The temperature drop in our 3D simulation of drying in SMS is shown in figure 15e-f. We can see the average and maximum temperature drops are $0.2K$ and $8.0K$, which are smaller than that in 2D simulation of $2.6K$ and $10.0K$. Especially for the average temperature drop, it is very small. In the work of Stadler & Carro (2016), they find that the temperature at the meniscus first increases by around $1.0K$ and then drop to up $5.0K$ in the water drying experiment in a two-layer structure ($60\mu m$ high) under the heating temperature of $76^\circ C$. The temperature variation is very similar to the average of maximum drop ($5.5K$) in our 3D simulation. For the average temperature drop, they find it is less than $1.0K$, which is also comparable with our 3D simulation.

We further investigate the change of liquid mass and evaporation rate with time. As shown in figure 15a, the evolution of the normalized liquid mass with time is quite similar in 2D, 3D and experiment. In figure 15b, we can see that the evaporation rate of our 3D simulation decreases more slowly than in the 2D simulation, and generally agrees better with the experiment. Especially after $t_N \approx 30$, when the evaporation rate only slightly decreases in the 3D simulation, but decreases much more significantly in 2D. The reason is, as explained in section 5.1, that more thermal energy is available in 3D for evaporation. For a more detailed comparison, we evaluate the relative errors of the liquid mass ($Err_m = (m(LBM) - m(exp))/m(exp)$) and evaporation rate ($Err_{Ep} = (Ep(LBM) - Ep(exp))/Ep(exp)$) for 2D and 3D simulations results, compared to experiment. For average relative errors of liquid mass and evaporation rate, they are 3.3%, 7.9% in 3D simulations, which are also smaller than 7.2%, 11.7% in 2D simulations. It is clear that the 3D simulation is generally more accurate quantitatively than the 2D one. However,

Figure 15: Comparison of a) liquid mass and b) evaporation rate between experiment, 2D and 3D T-EMRT-MP LBM simulation results in SMS; c) average temperature variation and d) maximum temperature variation between 2D and 3D T-EMRT-MP LBM simulation results in SMS. All variables are in physical units.

	Re_L	Re_V	Ca	$Pe_{L,T}$	$Pe_{V,m}$
experiment	0.014	0.006	3.51E-7	0.05	3.68E-3
3D LBM	0.450	0.105	6.08E-3	0.37	3.26E-3
mechanism	laminar flow	laminar flow	capillary force dominant	diffusion dominant	diffusion dominant

Table 3: Non-dimensional numbers for experiment and 3D LBM simulation in SMS

the computational cost in 3D simulation is 8.0 CPU hours with 8,800 processors, which is much higher than that in 2D simulation. Finally, the non-dimensional numbers for the 3D simulations are found in the similar regime as those of the experiments (Table 3).

In our 3D simulation, the liquid films adjacent to the plates are not seen since the contact angle is $\theta = 30^\circ$, which is not completely wetting. When we use a contact angle of $\theta = 0^\circ$, liquid films adjacent to the plates and the corners between the plates and pillars are seen at some time frames as shown in figure 16. However, the films do not last for a long time. The explanation is that, the evaporation is ongoing under the heating temperature of 50°C , which is much higher than ambient temperature and makes the evaporation much faster than the isothermal evaporation under ambient temperature. Apart from this, the strength of pumping effect also changes due to the varying of contact angle. The pumping effect is due to capillary pressure difference, i.e. $\sigma \cos \theta (1/r_2 - 1/r_1)$, where r_2 and r_1 are small and large pore spaces as shown in figure 7 and 11, respectively. With θ decreasing from 30° to 0° , the pumping effect is strengthened, leading to the

Figure 16: Liquid configuration at two different time frames ($t=48.30s$ and $t=128.84s$) with the zoom of films adjacent to plates and pillar corners. The contact angle is $\theta = 0^\circ$.

overall increase of evaporation rate. As a result, the total evaporation time with $\theta = 0^\circ$ is reduced to around 93.5% of that with $\theta = 30^\circ$ in our 3D simulations.

Overall, both 2D and 3D simulations capture the spiral evaporation route observed in the experiment. For quantitative results such as liquid mass and evaporation rate, the 3D simulation results are slightly better than the 2D results. In conclusion, 2D simulations are suitable for studying the evaporation pattern and rate in these quasi-two-dimensional micro-pillar cavities, while 3D simulations are more accurate in terms of quantitative analysis and simulated temperature field. The drawback of 3D simulation is that the computational cost is much higher compared to 2D. This means 2D simulations can be used for a quicker exploration of different micro-pillar configurations, while 3D can be used for a better prediction of the temperature field.

7. Conclusion

In this paper, non-isothermal liquid evaporation in specifically designed micro-pore structures is studied both experimentally and numerically. A hybrid thermal entropic multiple-relaxation-time multiphase lattice Boltzmann model (T-EMRT-MP LBM) is implemented and validated with droplet evaporation experiments to demonstrate the capability of simulating non-isothermal liquid evaporation. Then liquid evaporation in two micro pore structures, i.e. spiral-shaped and gradient-shaped micro-pillar cavities, referred to as SMS and GMS, is simulated. In SMS, the main evaporation front follows a spiral route while in GMS it moves layer by layer from large pillar distances to smaller ones, and both of them agree well with experiments. From the temperature field obtained from our T-EMRT-MP LBM simulation, we observed and explained latent heat effects at liquid-vapor interface (evaporative cooling) as well as heat conduction in liquid and vapor. Quantitatively, in both SMS and GMS the change of liquid mass with time coincides with experimental measurements. The evaporation rate is found to decrease with time mainly because of the reduction in liquid-vapor interface. In SMS, small peaks are observed in evaporation rate in both simulation and experiment, which are caused by evaporation of liquid film formed among pillars when main evaporation front passes the corner of the cavity. In GMS, the evaporation fluctuates reflecting the consecutive de-pinning of menisci at the evaporation front. The analysis of non-dimensional numbers such as Reynolds, capillary and Peclet numbers shows that, the internal liquid flow is in laminar flow regime and capillary forces are dominant over viscous forces leading to pinning of the menisci to the pillars. The simulation results demonstrate that our T-EMRT-MP LBM is able to capture the non-isothermal evaporation phenomena observed

in the experiments. Based on our numerical and experimental study, we find it is possible to control the evaporation route in pore structures at relatively high evaporation rate.

Acknowledgements

Swiss National Science Foundation (SNF, project No. 160189) is acknowledged for the financial support. Dr. Q.K. acknowledges the support from LANL’s LDRD Program and Institutional Computing Program. Dr. A.M.M. acknowledges the support from the computational resources at the Swiss National Super Computing Center CSCS (project No. s823).

Appendix A. How diffusive evaporation is considered in our model

We use a single component/specie two-phase model (liquid and vapor) to model the evaporation process. In our coupling model, we do not have an explicit equation for vapor diffusion (evaporation). The evaporation (mass transport) is induced by vapor pressure difference, which is controlled by temperature difference through equation of state (EoS). Under equilibrium state with saturation temperature T_{sat} and saturation pressure P_{sat} , there is no phase change between liquid and vapor. Once there is a temperature variation, the liquid and vapor tend to reach a new equilibrium state with different densities under new temperature. For example, if we heat up the liquid from T_1 to T_2 shown in figure 17, liquid density decreases from $\rho_{l,1}$ to $\rho_{l,2}$ while vapor density increases from $\rho_{v,1}$ to $\rho_{v,2}$ at the interface. The fluid pressure at T_2 is higher than that at T_1 , i.e. $P(T_2) > P(T_1)$. In this way, the vapor at the interface has a higher pressure (density) than that at the boundary. The pressure (density) difference drives the motion of vapor molecules. This process can be analogized to diffusion driven by concentration gradient, where pressure can be analogized to vapor partial pressure, while the vapor density analogized to vapor concentration. According to Fick’s law $J = D_v(d\varphi_v/dL_v)$, J is the diffusion flux with the unit of $mol/(m^2s)$ while φ_v is the vapor concentration with the unit of mol/m^3 . Since we care about the mass flux q with the unit of $kg/(m^2s)$, the Fick’s law is modified to be $q = D_v(d\rho_v/dL_v)$ with ρ_v represents the vapor density with the unit of kg/m^3 . The modified Fick’s law is used to calculate the vapor mass diffusion coefficient in our simulations shown in section 5 and 6. In fact, Cueto-felgueroso *et al.* (2018) also applied the same equation ($q = D_v(d\rho_v/dL_v)$) in their isothermal phase change model, and they have shown that it is sufficient to study liquid evaporation. In the future, we will improve our model by incorporating the effect of air (such as partial pressure, convection).

Appendix B. Single droplet evaporation in a closed cavity

A single droplet evaporating in a closed cavity is simulated and the results are compared with the diameter square law, as well as the results from Gong *et al.* (2018). As per in Gong *et al.* (2018), the droplet size is 65 lattices and located in the middle of a 2D square domain with $N_x \times N_y = 245 \times 245$. The density ratio of liquid and vapor is $\rho_l/\rho_v \approx 30$ with temperature ratio at $T/T_c = 0.75$, where T_c is the critical temperature. The droplet temperature is initially set as $T_d/T_c = 0.75$ and the surrounding vapor is $T_v/T_c = 0.86$.

Figure 17: The relation between pressure and volume of two-phase flow under different temperatures

Figure 18: Snapshots of droplet evaporating in a closed cavity at different normalized times t^*

Figure 19: Comparison of normalized diameter squared and error versus normalized time for T-EMRT-MP LBM results, LBM (Gong *et al.* 2018) results and the diameter square law.

All the surfaces of the domain are non-slip wall, and the wall temperature is set as $T_w/T_c = 0.86$ during the entire process. In this simulation, the thermal conductivity and heat capacity of liquid and vapor are both set as $\lambda = 0.4$ and $C_V = 120$. To compare our results with the Gong model (Gong *et al.* 2018), we use normalized time $t^* = t/t_{tot}$ and diameter square $D^2(t)/D_0^2$. The drying process in our simulation at different times are shown in figure 18, while the comparison is shown in figure 19. The error is calculated by simulated value minus analytical value of normalized diameter square, i.e. $Error = (D/D_0)^2(Sim.) - (D/D_0)^2(Ana.)$. From figure 19 we can see the error of our T-EMRT-MP LBM is always smaller than 0.014, while it can reach 0.040 for the Gong model. It is obvious that the agreement between our T-EMRT-MP LBM simulation and diameter square law is better than the Gong model.

Appendix C. Liquid evaporation in a capillary tube

To check the accuracy of our model for quasi-isothermal evaporation, we simulate the evaporation in a capillary tube and compared with the analytical solution. We assume a capillary tube with length of 3.2mm and width of 0.32mm, and the left side is open for evaporation as shown in figure 20. According to Cueto-felgueroso *et al.* (2018), the analytical solution of the meniscus distance from outlet boundary with time is written as $x_m(t) = \left(2D_v \frac{\rho_v^* - \rho_v^{out}}{\rho_l^* - \rho_v^*}\right)^{1/2} t^{1/2}$, where $\rho_l^*, \rho_v^*, \rho_v^{out}$ represent the liquid density vapor density at meniscus and outlet boundary. We mention that, this analytical solution does not consider the effect of contact angle θ . Considering the evaporation is under the temperature of $55^\circ C$, and the environment temperature is $22^\circ C$ with relative humidity of 36%. Then we get the parameters as: $D_v = 3.05e - 5 m^2/s$, $\rho_l^* = 985.7 kg/m^3$, $\rho_v^* = 0.126 kg/m^3$ and $\rho_v^{out} = 0.0454 kg/m^3$. Thus the analytical solution is simply written as: $x_m(t) = 6.63 \times 10^{-5} \times t^{1/2} m$. The total evaporation time and average velocity of meniscus are calculated as $t_{tot} = 2328.9s$ and $\bar{u}_m = 1.37 \times 10^{-6} m/s$.

In our simulation, we set liquid and vapor outlet temperatures as $T_l = 0.80T_c$ and $T_v^{out} = 0.75T_c$ in order to keep the same temperature difference as in the above case, i.e. $\frac{T_l - T_v^{out}}{T_c} = 0.80 - 0.75 = \frac{55-22}{647} = 0.05$. We simulate the evaporation with three different contact angles of $\theta = 40^\circ, 90^\circ, 130^\circ$, varying from hydrophilic to hydrophobic. Our simulations are done with hybrid LBM, which is a mesoscopic numerical model with the units being lattice units instead of physical units. To compare the numerical modelling with experiments, we have to convert the lattice units (length and time) to physical ones. For the time unit conversion, we use non-dimensional time $t^* = \frac{u_0 \times t}{L_{tube}}$ as the medium, where u_0 is the characteristic velocity of the meniscus and L_{tube} is the length of the tube. In physical units, the characteristic velocity is derived as: $u_{0,p} = D_v \frac{\rho_v^* - \rho_v^{out}}{\rho_l^* - \rho_v^*} \frac{1}{dx}$. If we consider the average velocity as the characteristic velocity, then $dx = L_{tube,p}/2$. Thus the characteristic velocity is $u_{0,p} = D_v \frac{\rho_v^* - \rho_v^{out}}{\rho_l^* - \rho_v^*} \frac{2}{L_{tube,p}}$. In lattice units, the corresponded characteristic velocity is: $u_{0,l} = \sqrt{\frac{2(p_v^* - p_v^{out})}{\rho_v^*} \frac{\rho_v^{out}}{\rho_l^*}}$. In this way, the non-dimensional time for lattice and physical units are $t_l^* = \frac{u_{0,l} \times t_l}{L_{tube,l}}$ and $t_p^* = \frac{u_{0,p} \times t_p}{L_{tube,p}}$. In simulations and experiments, the non-dimensional time for each should be identical, i.e. $t_l^* = t_p^*$. Then the dimensional time in physical units can be calculated as: $t_p = \frac{u_{0,l} L_{tube,p}}{u_{0,p} L_{tube,l}} t_l$. For the non-dimensional length, we use total length of tube as the medium, i.e. $x^* = \frac{x}{L_{tube}}$. Then the non-dimensional lengths in lattice and physical units are $x_l^* = \frac{x_l}{L_{tube,l}}$ and

Figure 20: Schematic illustration of liquid drying in the capillary tube

Figure 21: Comparison of meniscus position of liquid drying in the capillary tube between analytical solution and hybrid LBM simulations with three different contact angles

$x_p^* = \frac{x_p}{L_{tube,p}}$. Similarly, with the equality of the non-dimensional lengths $x_l^* = x_p^*$, we get $x_p = \frac{L_{tube,p}}{L_{tube,l}} x_l$.

Then we can plot the relation between x_p and t_p to compare with the analytical solution $x_m(t) = \left(2D_v \frac{\rho_v^* - \rho_v^{out}}{\rho_l^* - \rho_v^*}\right)^{1/2} t^{1/2}$ mentioned above. From figure 21 we can see that, our simulation results agree reasonably well with analytical solution. The drying times with contact angles of $\theta = 40^\circ, 90^\circ, 130^\circ$ are 2439s, 2340s and 2209s, indicating the small effect of contact angle on evaporation rate. With the increase of contact angles, the fluid-solid interaction force is getting smaller and the meniscus changes from concave to convex, which increases a little bit of the evaporation rate. That is why the evaporation time is getting smaller with the increase of contact angles.

Appendix D. Conversion from lattice to physical units

To better compare our simulation results with experimental ones, we do the conversions from lattice units to physical ones similar to that in Appendix C. We compare the liquid mass, evaporation rate and interface area with time. Then the dimensional time in physical units is calculated as $t_p = \frac{\overline{u_{m,l}} L_p}{\overline{u_{m,p}} L_l} t_l$, where $\overline{u_{m,l}}$ and $\overline{u_{m,p}}$ are the average velocities of main liquid-vapor meniscus, L_l and L_p (figure 4) are the characteristic moving distance of the main liquid-vapor meniscus in simulation and experiment. For the liquid mass left in the micro-pore structures, the corresponded conversion is $m_p = \frac{m_{0,p}}{m_{0,l}} m_l$ with $m_l = \rho_{l,l} A_{l,l} H_l$, $m_{0,l} = \rho_{l,l} A_{0,l} H_l$, $m_{0,p} = \rho_{l,p} A_{0,p} H_p$, where $m_p, m_{0,p}, \rho_{l,p}, A_{0,p}$ and

$m_l, m_{0,l}, \rho_{l,l}, A_{0,l}$ are liquid mass during drying, initial liquid mass, liquid density, initial liquid area in physical and lattice units. $A_{l,l}$ is liquid area in lattice units during drying. H_p, H_l are the heights of liquid in the micro-pore structure in physical and lattice units, and we assume $H_l = \frac{L_l}{L_p} H_p$. With the converted liquid mass and time in physical units, we can calculate the evaporation rate in physical units as $Ep_p = \left| \frac{\Delta m_p}{\Delta t_p} \right|$. Similarly, we can convert the interfacial area from lattice units I_l to physical units I_p with $I_l = \frac{I_{0,l}}{I_{0,p}} I_p$ where $I_{0,l}$ and $I_{0,p}$ are initial interfacial area in lattice and physical units. We also do it for temperature. The critical temperature in simulations and experiment are $T_{cl} = 0.0943$ and $T_{cp} = 647K$. The temperature variation to critical temperature should be the same in both physical and lattice units, namely $dT_p/T_{cp} = dT_l/T_{cl}$. Thus the temperature variation in physical units can be given as $dT_p = T_{cp} * dT_l/T_{cl}$, in which $dT_l = T_l - T_{l,0}$ and $T_{l,0}$ is the initial temperature in simulations. The comparison of liquid mass, evaporation rate, liquid-vapor interface and temperature with converted units are compared in section 5 and 6.

REFERENCES

- BLUNT, MARTIN J, BIJELJIC, BRANKO, DONG, HU, GHARBI, OUSSAMA, IGLAUER, STEFAN, MOSTAGHIMI, PEYMAN, PALUSZNY, ADRIANA & PENTLAND, CHRISTOPHER 2013 Advances in Water Resources Pore-scale imaging and modelling. *Advances in Water Resources* **51**, 197–216.
- BOEK, EDO S. & VENTUROLI, MADDALENA 2010 Lattice-Boltzmann studies of fluid flow in porous media with realistic rock geometries. *Computers and Mathematics with Applications* **59** (7), 2305–2314.
- BOLES, MICHAEL A., ENGEL, MICHAEL & TALAPIN, DMITRI V. 2016 Self-assembly of colloidal nanocrystals: From intricate structures to functional materials. *Chemical Reviews* **116** (18), 11220–11289.
- BÖSCH, FABIAN, CHIKATAMARLA, SHYAM S. & KARLIN, ILYA V. 2015 Entropic multirelaxation lattice Boltzmann models for turbulent flows. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **92** (4), 1–15, arXiv: 1507.02518.
- BRUNSCHWILER, THOMAS, ZÜRCHER, JONAS, DEL CARRO, LUCA, SCHLOTTIG, GERD, BURG, BRIAN, ZIMMERMANN, SEVERIN, ZSCHENDERLEIN, UWE, WUNDERLE, BERNHARD, SCHINDLER-SAEFKOW, FLORIAN & STÄSSLE, RAHEL 2016 Review on Percolating and Neck-Based Underfills for Three-Dimensional Chip Stacks. *Journal of Electronic Packaging* **138** (4), 041009.
- CHEN, CHEN, DURU, PAUL, JOSEPH, PIERRE, GEOFFROY, SANDRINE & PRAT, MARC 2017 Control of evaporation by geometry in capillary structures. from confined pillar arrays in a gap radial gradient to phyllotaxy-inspired geometry. *Scientific Reports* **7** (1), 1–8.
- CHEN, C., JOSEPH, P., GEOFFROY, S., PRAT, M. & DURU, P. 2018 Evaporation with the formation of chains of liquid bridges. *Journal of Fluid Mechanics* **837**, 703–728.
- CHEN, LI, KANG, QINJUN, MU, YUTONG, HE, YA LING & TAO, WEN QUAN 2014 A critical review of the pseudopotential multiphase lattice Boltzmann model: Methods and applications. *International Journal of Heat and Mass Transfer* **76**, 210–236.
- CHEN, LI, LUAN, HUI-BAO, HE, YA-LING & TAO, WEN-QUAN 2012 Pore-scale flow and mass transport in gas diffusion layer of proton exchange membrane fuel cell with interdigitated flow fields. *International Journal of Thermal Sciences* **51**, 132–144.
- CHIKATAMARLA, S. S., ANSUMALI, S. & KARLIN, I. V. 2006 Entropic lattice Boltzmann models for hydrodynamics in three dimensions. *Physical Review Letters* **97** (1), 1–4.
- CUETO-FELGUEROSO, LUIS, FU, XIAOJING & JUANES, RUBEN 2018 PHYSICAL REVIEW FLUIDS **3**, 084302 (2018) Pore-scale modeling of phase change in porous media **084302**, 1–28.
- DASH, SUSMITA & GARIMELLA, SURESH V. 2013 Droplet evaporation dynamics on a superhydrophobic surface with negligible hysteresis. *Langmuir* **29** (34), 10785–10795.

- DASH, SUSMITA & GARIMELLA, SURESH V. 2014 Droplet evaporation on heated hydrophobic and superhydrophobic surfaces. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **89** (4), 1–8.
- DEFRAEYE, THIJS 2014 Advanced computational modelling for drying processes - A review. *Applied Energy* **131**, 323–344.
- DEFRAEYE, THIJS, AREGAWI, WONDWOSEN, SANEINEJAD, SABA, VONTOBEL, PETER, LEHMANN, EBERHARD, CARMELIET, JAN, VERBOVEN, PIETER, DEROME, DOMINIQUE & NICOLAÏ, BART 2013 Novel Application of Neutron Radiography to Forced Convective Drying of Fruit Tissue. *Food and Bioprocess Technology* **6** (12), 3353–3367.
- DEFRAEYE, THIJS, HOUVENAGHEL, GEERT, CARMELIET, JAN & DEROME, DOMINIQUE 2012 Numerical analysis of convective drying of gypsum boards. *International Journal of Heat and Mass Transfer* **55** (9–10), 2590–2600.
- DUNN, G. J., WILSON, S. K., DUFFY, B. R., DAVID, S. & SEFIANE, K. 2009 The strong influence of substrate conductivity on droplet evaporation. *Journal of Fluid Mechanics* **623**, 329.
- FANTINEL, PAOLO, BORGMAN, OSHRI, HOLTZMAN, RAN & GOEHRING, LUCAS 2017 Drying in a microfluidic chip: Experiments and simulations. *Scientific Reports* **7** (1), 1–12.
- FATT, IRVING 1956 The Network Model of Porous Media. *Petroleum Transactions, AIME* **207**, 144–181.
- GHASSEMI, ALI & PAK, ALI 2011 Numerical study of factors influencing relative permeabilities of two immiscible fluids flowing through porous media using lattice Boltzmann method. *Journal of Petroleum Science and Engineering* **77** (1), 135–145.
- GONG, W, YAN, Y Y, CHEN, S & WRIGHT, E 2018 International Journal of Heat and Mass Transfer A modified phase change pseudopotential lattice Boltzmann model. *International Journal of Heat and Mass Transfer* **125**, 323–329.
- HAMON, CYRILLE, POSTIC, MARIE, MAZARI, ELSA, BIZIEN, THOMAS, DUPUIS, CHRISTOPHE, EVEN-HERNANDEZ, PASCALE, JIMENEZ, ANGELA, COURBIN, LAURENT, GOSSE, CHARLIE, ARTZNER, FRANCK & MARCHI-ARTZNER, VALÉRIE 2012 Three-dimensional self-assembling of gold nanorods with controlled macroscopic shape and local smectic B order. *ACS Nano* **6** (5), 4137–4146.
- HIRT, C. W. & NICHOLS, B. D. 1981 Volume of fluid (VOF) method for the dynamics of free boundaries. *Journal of Computational Physics* **39** (1), 201–225, arXiv: 0924-0136(97)00224-0.
- HUANG, HAIBO, LI, ZHITAO, LIU, SHUAISHUAI & LU, XI-YUN 2009 Shan-and-Chen-type multiphase lattice Boltzmann study of viscous coupling effects for two-phase flow in porous media. *International Journal for Numerical Methods in Fluids* (October 2007), 601–629, arXiv: fld.1.
- IRAWAN, A. 2006 Isothermal Drying of Pore networks : Influence of Pore Structure on Drying Kinetics. *Otto-von-Guericke-University of Magdeburg PhD thesis* (June).
- KANG, QINJUN, CHEN, LI, VALOCCHI, ALBERT J & VISWANATHAN, HARI S 2014 Pore-scale study of dissolution-induced changes in permeability and porosity of porous media. *Journal of Hydrology* **517**, 1049–1055.
- KANG, QINJUN, ZHANG, DONGXIAO & CHEN, SHIYI 2002 Displacement of a two-dimensional immiscible droplet in a channel. *Physics of Fluids* **14** (9), 3203–3214.
- KARLIN, I. V., BÖSCH, F. & CHIKATAMARLA, S. S. 2014 Gibbs' principle for the lattice-kinetic theory of fluid dynamics. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **90** (3), 1–5.
- KARLIN, I. V, FERRANTE, A & ÖTTINGER, H. C 1999 Perfect entropy functions of the Lattice Boltzmann method. *Europhysics Letters (EPL)* **47** (2), 182–188.
- LAURINDO, JOAO BORGES & PRAT, MARC 1998 Numerical and experimental network study of evaporation in capillary porous media. Drying rates. *Chemical Engineering Science* **51** (23), 5171–5185.
- LAW, C. K. 1982 Recent advances in droplet vaporization and combustion. *Progress in Energy and Combustion Science* **8** (3), 171–201.
- LEE, TAEHUN & LIN, CHING LONG 2005 A stable discretization of the lattice Boltzmann equation for simulation of incompressible two-phase flows at high density ratio. *Journal of Computational Physics* **206** (1), 16–47.

- LI, HUINA, PAN, CHONGXUN & MILLER, CASS T. 2005 Pore-scale investigation of viscous coupling effects for two-phase flow in porous media. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **72** (2), 1–14.
- LI, Q., KANG, Q. J., FRANCOIS, M. M., HE, Y. L. & LUO, K. H. 2015 Lattice Boltzmann modeling of boiling heat transfer: The boiling curve and the effects of wettability. *International Journal of Heat and Mass Transfer* **85**, 787–796.
- LI, Q., LUO, KAI H., KANG, QINJUN, HE, Y. L., CHEN, Q. & LIU, Q. 2016a Lattice Boltzmann methods for multiphase flow and phase-change heat transfer. *Progress in Energy and Combustion Science* **52** (0), 62–105, arXiv: 1508.00940.
- LI, QING, ZHOU, P. & YAN, H. J. 2016b Pinning-Depinning Mechanism of the Contact Line during Evaporation on Chemically Patterned Surfaces: A Lattice Boltzmann Study. *Langmuir* **32** (37), 9389–9396, arXiv: 1609.0182.
- LI, QING, ZHOU, P. & YAN, H. J. 2017 Improved thermal lattice Boltzmann model for simulation of liquid-vapor phase change. *Physical Review E* **96** (6), arXiv: 1709.04400.
- LIU, HAIHU, KANG, QINJUN, LEONARDI, CHRISTOPHER R., SCHMIESCHEK, SEBASTIAN, NARVÁEZ, ARIEL, JONES, BRUCE D., WILLIAMS, JOHN R., VALOCCHI, ALBERT J. & HARTING, JENS 2016 Multiphase lattice Boltzmann simulations for porous media applications – a review. *computational geosciences* pp. 777–805, arXiv: 1404.7523.
- LIU, HAIHU, VALOCCHI, ALBERT J., ZHANG, YONGHAO & KANG, QINJUN 2013 Phase-field-based lattice Boltzmann finite-difference model for simulating thermocapillary flows. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **87** (1), 1–13.
- LIU, HAIHU, VALOCCHI, ALBERT J., ZHANG, YONGHAO & KANG, QINJUN 2014 Lattice Boltzmann phase-field modeling of thermocapillary flows in a confined microchannel. *Journal of Computational Physics* **256**, 334–356, arXiv: 0812.0143v2.
- LIU, HAIHU, ZHANG, YONGHAO & VALOCCHI, ALBERT J. 2015 Lattice boltzmann simulation of immiscible fluid displacement in porous media: Homogeneous versus heterogeneous pore network. *Physics of Fluids* **27** (5).
- METZGER, THOMAS & TSOTSAS, EVANGELOS 2008 Viscous stabilization of drying front: Three-dimensional pore network simulations. *Chemical Engineering Research and Design* **86** (7), 739–744.
- OSHER, STANLEY & FEDKIW, RONALD P. 2001 Level Set Methods: An Overview and Some Recent Results. *Journal of Computational Physics* **169** (2), 463–502.
- PILLAI, K. M., PRAT, M. & MARCOUX, M. 2009 A study on slow evaporation of liquids in a dual-porosity porous medium using square network model. *International Journal of Heat and Mass Transfer* **52** (7-8), 1643–1656.
- PRAT, M. 2007 On the influence of pore shape, contact angle and film flows on drying of capillary porous media. *International Journal of Heat and Mass Transfer* **50** (7-8), 1455–1468.
- QIN, F., MOQADDAM, A. MAZLOOMI, KANG, Q., D.DEROME & CARMELIET, J. 2018 Entropic multiple-relaxation-time multirange pseudopotential lattice Boltzmann model for two-phase flow. *Physics of Fluids* **032104**.
- SAXTON, M. A., WHITELEY, J. P., VELLA, D. & OLIVER, J. M. 2016 On thin evaporating drops: When is the d2-law valid? *Journal of Fluid Mechanics* **792**, 134–167.
- SBRAGAGLIA, M., BENZI, R., BIFERALE, L., SUCCI, S., SUGIYAMA, K. & TOSCHI, F. 2007 Generalized lattice Boltzmann method with multirange pseudopotential. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics* **75** (2), 1–13, arXiv: 0611014.
- SHAERI, MOHAMMAD REZA, BEYHAGHI, SAMAN & PILLAI, KRISHNA M. 2013 On applying an external-flow driven mass transfer boundary condition to simulate drying from a pore-network model. *International Journal of Heat and Mass Transfer* **57** (1), 331–344.
- STÄDLER, ROMAN & CARRO, LUCA DEL 2016 Study of capillary bridging induced self-assembly to improve robustness of neck-based thermal underfill. *ETHz master thesis*.
- STÄDLER, ROMAN, CARRO, LUCA D., ZURCHER, JONAS, SCHLOTTIG, GERD, STUDART, ANDRE R. & BRUNSCHWILER, THOMAS 2017 Direct investigation of microparticle self-assembly to improve the robustness of neck formation in thermal underfills. *IEEE ITherm Conference* pp. 167–173.
- STALDER, AURÉLIEN F., MELCHIOR, TOBIAS, MÜLLER, MICHAEL, SAGE, DANIEL, BLU, THIERRY & UNSER, MICHAEL 2010 Low-bond axisymmetric drop shape analysis for

- surface tension and contact angle measurements of sessile drops. *Colloids and Surfaces A: Physicochemical and Engineering Aspects* **364** (1-3), 72–81.
- STAUBER, J. M., WILSON, S. K., DUFFY, B. R. & SEFIANE, K. 2014 On the lifetimes of evaporating droplets. *Journal of Fluid Mechanics* **744**, R2.
- SUKOP, MICHAEL C. & OR, DANI 2003 Invasion percolation of single component, multiphase fluids with lattice Boltzmann models. *Physica B: Condensed Matter* **338** (1-4), 298–303.
- SURASANI, V. K., METZGER, T. & TSOTSAS, E. 2008 Consideration of heat transfer in pore network modelling of convective drying. *International Journal of Heat and Mass Transfer* **51** (9-10), 2506–2518.
- SURASANI, V. K., METZGER, T. & TSOTSAS, E. 2009 A Non-isothermal pore network drying model with gravity effect. *Transport in Porous Media* **80** (3), 431–439.
- SURASANI, V. K., METZGER, T. & TSOTSAS, E. 2010 Drying simulations of various 3D pore structures by a nonisothermal pore network model. *Drying Technology* **28** (5), 615–623.
- SUSSMAN, M., SMEREKA, P. & OSHER, S. 1994 A Level Set Approach for Computing Solutions to Incompressible Two-Phase Flow, arXiv: 1994.
- TASLIMI TALEGHANI, SARA & DADVAR, MITRA 2014 Two dimensional pore network modelling and simulation of non-isothermal drying by the inclusion of viscous effects. *International Journal of Multiphase Flow* **62**, 37–44.
- VORHAUER, NICOLE, METZGER, THOMAS & TSOTSAS, EVANGELOS 2011 on the Influence of Temperature Gradients on Drying of Pore Networks. *European Drying Conference - EuroDrying'2011* (October), 26–28.
- VORHAUER, N., TRAN, Q. T., METZGER, T., TSOTSAS, E. & PRAT, M. 2013 Experimental Investigation of Drying in a Model Porous Medium: Influence of Thermal Gradients. *Drying Technology* **31** (8), 920–929.
- VORHAUER, N., WANG, Y. J., KHARAGHANI, A., TSOTSAS, E. & PRAT, M. 2015 Drying with Formation of Capillary Rings in a Model Porous Medium. *Transport in Porous Media* **110** (2), 197–223.
- WODLEI, F., SEBILLEAU, J., MAGNAUDET, J. & PIMIENTA, V. 2018 Marangoni-driven flower-like patterning of an evaporating drop spreading on a liquid substrate. *Nature Communications* **9** (1), 1–12.
- YIOTIS, A G, BOUDOUVIS, A G, STUBOS, A. K., TSIMPANOIANNIS, I. N. & YORTSOS, Y. C. 2004 Effect of Liquid Films on the Drying of Porous Media **50** (11), 2721–2737.
- YIOTIS, ANDREAS G., TSIMPANOIANNIS, IOANNIS N., STUBOS, ATHANASSIOS K. & YORTSOS, YANNIS C. 2006 Pore-network study of the characteristic periods in the drying of porous materials. *Journal of Colloid and Interface Science* **297** (2), 738–748.
- YIOTIS, ANDREAS G., TSIMPANOIANNIS, IOANNIS N., STUBOS, ATHANASSIOS K. & YORTSOS, YANNIS C. 2007 Coupling between external and internal mass transfer during drying of a porous medium. *Water Resources Research* **43** (6), 1–12.
- YU, Y., LI, Q., ZHOU, CHEN Q., ZHOU, P. & YAN, H. J. 2017 Investigation of droplet evaporation on heterogeneous surfaces using a three-dimensional thermal multiphase lattice Boltzmann model. *Applied Thermal Engineering* **127**, 1346–1354.
- YUAN, PENG & SCHAEFER, LAURA 2006 Equations of state in a lattice Boltzmann model. *Physics of Fluids* **18** (4).
- ZHANG, CHAOYANG, HONG, FANGJUN & CHENG, PING 2015 Simulation of liquid thin film evaporation and boiling on a heated hydrophilic microstructured surface by Lattice Boltzmann method. *International Journal of Heat and Mass Transfer* **86**, 629–638.
- ZURCHER, JONAS, CHEN, XI, BURG, BRIAN R., ZIMMERMANN, SEVERIN, STRAESSLE, RAHEL, STUART, ANDRE R. & BRUNSCHWILER, THOMAS 2016 Enhanced percolating thermal underfills achieved by means of nanoparticle bridging necks. *IEEE Transactions on Components, Packaging and Manufacturing Technology* **6** (12), 1785–1795.