

Molecular water layer evaporation & condensation

Citation for published version (APA):

Wolf, M. C. W., Frijns, A. J. H., Gaastra - Nedea, S. V., & Enright, R. (2017). Molecular water layer evaporation & condensation. In *Proceedings of the 2nd MIGRATE Workshop, June 29-30, 2017, Sofia, Bulgaria* (pp. 47-48). Article 154795.

Document status and date:

Published: 29/06/2017

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
- The final author version and the galley proof are versions of the publication after peer review.
- The final published version features the final layout of the paper including the volume, issue and page numbers.

[Link to publication](#)

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal.

If the publication is distributed under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license above, please follow below link for the End User Agreement:

www.tue.nl/taverne

Take down policy

If you believe that this document breaches copyright please contact us at:

openaccess@tue.nl

providing details and we will investigate your claim.

MIGRATE2017:154795

MOLECULAR WATER LAYER EVAPORATION & CONDENSATION

M.C.W. Wolf ^{*1,2}, A.J.H. Frijns ², S.V. Nedea ², Ryan Enright ¹¹Nokia Bell Labs, Blanchardstown Business & Technology Park Dublin, D15 Y6NT Ireland²Eindhoven University of Technology, PO Box 513, 5600MB Eindhoven, the Netherlands

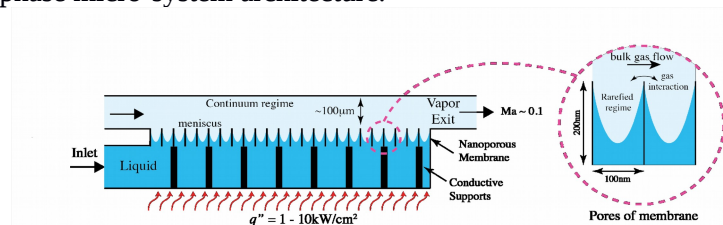
KEY WORDS

Molecular dynamics, nanopore evaporation, two-phase cooling

ABSTRACT

The past decade has seen a considerable growth in portable devices with mobile connectivity. This growth has been enabled by the development of high capacity telecommunication networks globally. Individuals require high data transfer capabilities to remotely stream large information sets (i.e. HD video) and this is leading to greater demands for next generation networks (i.e. 5G). To ensure this growth continues, hardware devices must be smaller, more energy-efficient and provide greater functionality. This requirement poses a thermal management challenge, increasing heat transfer density significantly. Novel materials and cooling methods, which are engineered at the micro- and nanoscale, are necessary to address this.

The overall aim of this project is to examine and maximize the heat transfer performance capabilities in an enclosed two-phase micro-system architecture.

**Figure 1:** Nanopore evaporation

A very promising cooling technique for the increasing heat transfer density is the method depicted in Fig. 1. In this two-phase cooling system, the liquid phase evaporates from the nanopores to the gas phase [1]. The latent heat of vaporization is the dominant mode of heat transfer while the nanopore geometry generates the requisite capillary pressure to drive the liquid flow to the heat source. This will be studied numerically (to increase the fundamental understanding of the phenomena) and be used to inform detailed experiments and system level design. Therefore, various solids (Si, SiO₂,...) , gases (Ar, H₂O, N₂,...) and rarefaction levels will be studied numerically.

In order to study the two-phase cooling system, we start with a simplified model of evaporation and condensation of a water layer system as shown in Fig. 2. We use Molecular Dynamics to investigate different properties of the simulation such as the temperature profile, heat flux, velocity distribution, water molecule orientation (WMO) [4] and the density distribution.

1* Corresponding author

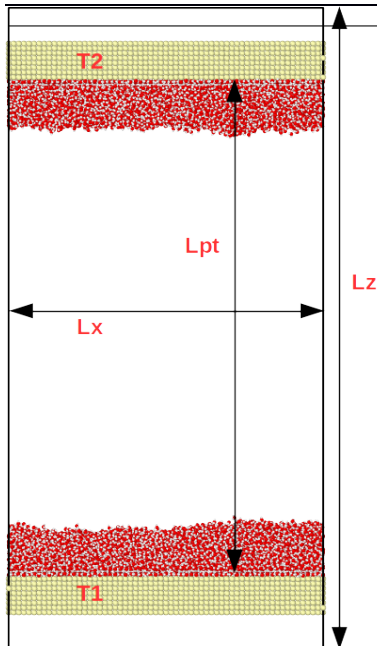


Figure 2: Simulation model for evaporation and condensation of a water layer

The dimensions of the simulation model are $L_x, L_y = 121 \text{ \AA}$, $L_z = 260 \text{ \AA}$ and $L_{pt} = 200 \text{ \AA}$. The temperature at the bottom and top walls are kept constant using a Nose-Hoover thermostat with $T_1=368\text{K}$ and $T_2=278\text{K}$. Periodic boundary conditions are applied in x, y and z direction. The water molecules are modeled using the TIP4P/2005 model [2] and the interaction between the 8 layers of platinum atoms are modeled using harmonic springs [3].

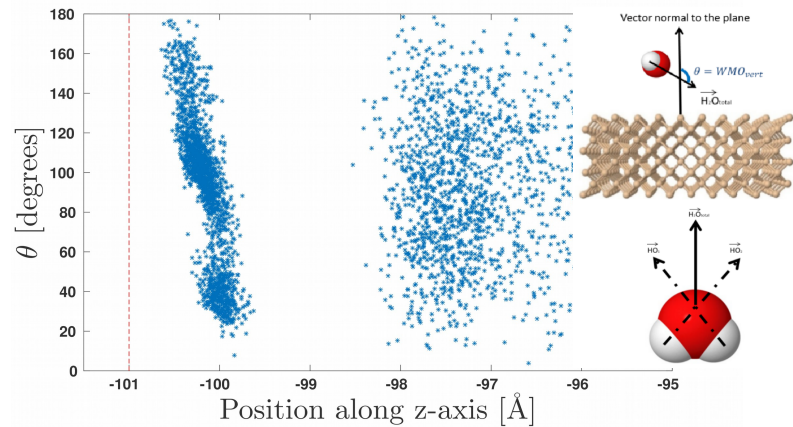


Figure 3: WMO near the bottom wall. Red line: begin of the bottom wall. Right insert: definition of water molecule orientation (WMO).

The results obtained so far are the WMO and the density distribution. It is observed in Fig. 3 that there exists a preferred water molecule orientation around 80° - 120° and 40° near the bottom wall. A similar observation can be made near the upper wall. In the bulk no preferred WMO is observed. This could influence the liquid-vapor interface and evaporation.

The density distribution along the z -axis shown in Fig. 4 indicates the high density in the walls and a decay near the liquid vapor interface.

The temperature profile, which is under investigation at the moment, will give us the opportunity to see possible temperature jumps near the solid-liquid and/or liquid/vapor interface and thereby provide us detailed information on the evaporation resistances.

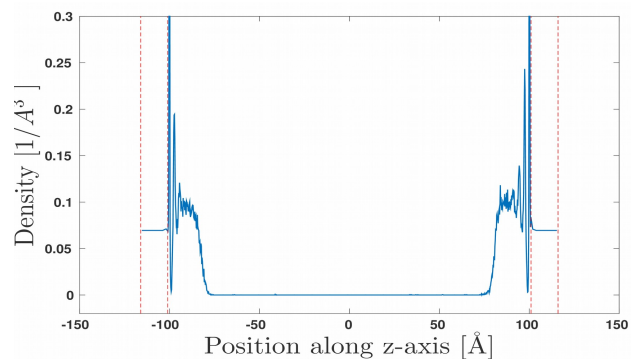


Figure 4: Density distribution along the z -axis. Red lines indicate the walls

Acknowledgements

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 643095.

References and Citations

- [1] D.F. Hanks (2016). Evaporation from Nanoporous Membranes for High Heat Flux Thermal Management. PhD thesis, MIT
- [2] Orsi, M. (2014). Comparative assessment of the ELBA coarse-grained model for water. *Molecular Physics*, **112(11)**, 1566-1576.
- [3] D.Torri and T.Ohara (2007). Molecular dynamics study on ultrathin liquid water film sheared between platinum solid walls: Liquid structure and energy and momentum transfer. *J. Chem. Phys*, **126(15)**:154706.
- [4] J. Kim (2014). Molecular Models for Water Vapor Flows in Silica Nanopores. PhD thesis, Eindhoven University of Technology