Off-lattice Monte-Carlo Approach for Studying Nucleation and Evaporation Phenomena at the Molecular Scale

Panagiotis E. Theodorakis[1], Jongjie Wang[1], Aqiang Chen[2], Bin Liu[2]

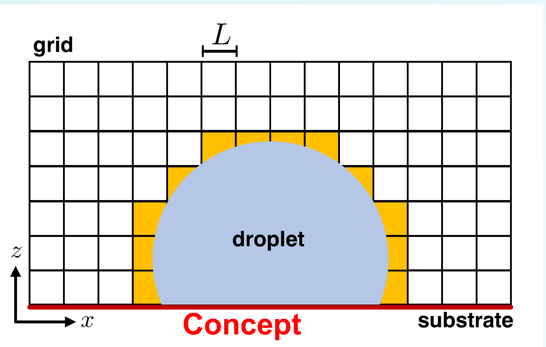
[1]Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warsaw, Poland

[2]Tianjin Key Laboratory of Refrigeration Technology, Tianjin University of Commerce, Tianjin 300134, China

Introduction

Key Concept: Droplet nucleation and evaporation phenomena are ubiquitous in nature and relevant for many practical applications on earth and is space.
Aim: Developing a computational framework that allows for the simulation of nucleation and evaporation phenomena at the molecular scale
Applications: Phase-change cooling, boiling heat transfer and others.

Model and Methodology

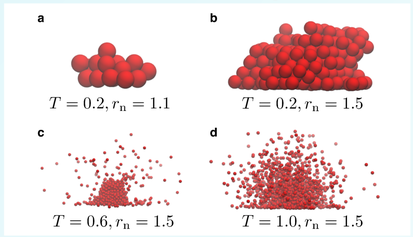


Concept

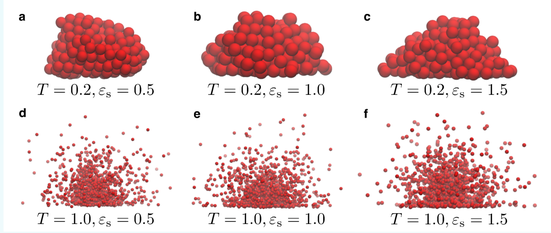
Model: Here, a standard Lennard-Jones (LJ) 12-6 fluid and a 9-3 LJ potential for the smotth and unstructured substrate is used for demonstrating the method.
Method: Combination of Monte Carlo techniques and the Volume-of-Fluid (VOF) method for tracking the interface.
Parameters: Temperature (T), chemical potential (μ), interaction between the fluid and the substrate (ε_s), size of the cells (L), cut-off distance (r_n) from the liquid–vapour (LV) surface, density of the cell (ρ_c).

Results

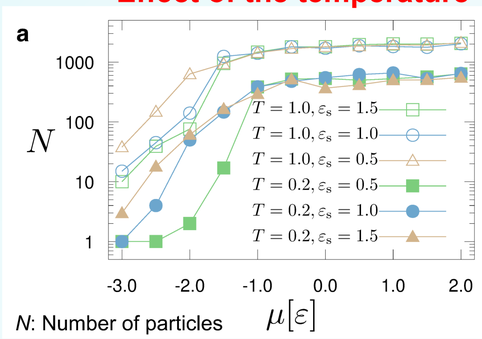
Effect of the temperature



Effect of the interaction with the substrate

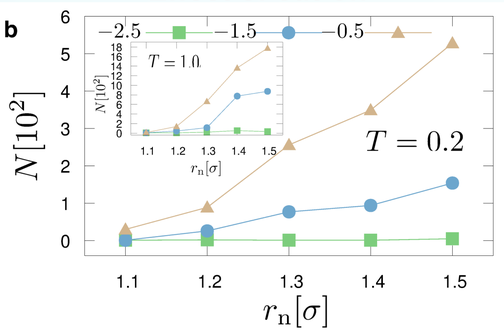


Effect of the temperature

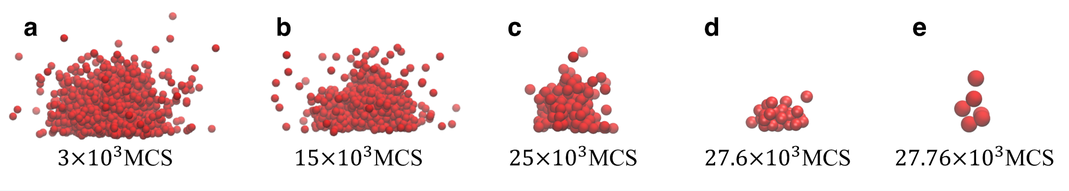


N: Number of particles

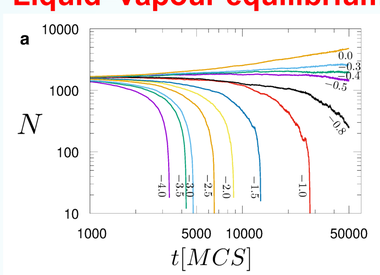
Effect of cut-off



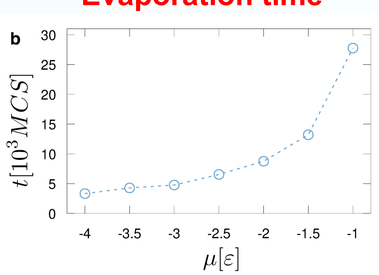
Droplet Evaporation (Time Evolution)



Liquid–vapour equilibrium

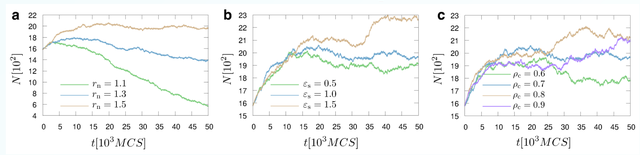


Evaporation time



Results

Cut-off should be kept the same



Liquid-vapour equilibrium for different sets of parameters

Conclusions

- A new molecular approach for investigating nucleation and evaporation phenomena.
- The method is based on the Monte Carlo method and the VOF method.
- We have analysed the dependence of the model on its parameters
- We have provided various examples and shown the possibility of reaching the liquid vapour equilibrium
- Vapour particles far from the LV surface are not required in the simulation, which increases the computational efficiency of the model.

References

1. P.E. Theodorakis, J. Wang, A. Chen, B. Liu, *Materials* **14**, 2092 (2021)

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. 778104. This research was supported in part by PLGrid Infrastructure.