Proceedings of the Canadian Society for Mechanical Engineering International Congress 2022
CSME Congress 2022
June 5-8, 2022, Edmonton, AB, Canada

Molecular dynamics investigations on liquid bridges formed between heterogeneous surfaces

A. Khalajiolyaie[1], C. Jian[1*]
Mechanical Engineering, York University, Toronto, Canada

*cuiying.jian@lassonde.yorku.ca

ABSTRACT

In the literature, most studies performed on liquid bridges were focused on homogeneous surfaces. However, understanding the behavior of liquid between heterogeneous surfaces is of great importance for applications in several industrial technologies, such as biomedicine and microfluidics. Therefore, this study aims to simulate the synergistic effects of hydrophobic and hydrophilic surfaces on the contact angle between water droplets and surfaces. Four models were constructed, where a single water droplet was placed between two surfaces of different properties: a) upper surface: hydrophilic, and bottom one: hydrophobic; b) upper surface: hydrophobic, and bottom one: hydrophilic; c) for both upper and bottom surfaces: half is hydrophilic, and half is hydrophobic; d) upper surface: the right half is hydrophobic and the left half is hydrophilic, and bottom surface: the right half is hydrophilic, and the left half is hydrophobic. Wettability is the balance of interfacial interactions for a system with different phases. From a thermodynamic point of view, such balances can be investigated by using Young's equation to calculate contact angles. Thus, contact angles for the aforementioned four modes were calculated to examine the behavior of liquid bridges. When the water droplet was placed between two heterogeneous surfaces, four angles were created; two contact angles were formed between the droplet and the bottom surface, and the other two angles were formed between the droplet and the upper surface. It was found that larger contact angles between the water droplet and surfaces lead to less tendency for wettability. The largest contact angle (84°) was obtained for the hydrophobic parts of each surface due to the lowest tendency to be wetted, and the smallest contact angle (28°) was obtained for the hydrophilic parts because of the similar wettability of water and hydrophilic surfaces. The results further revealed that a liquid bridge was formed in the steady-state, when the upper-right and bottom-left surfaces are hydrophobic and the other parts of surfaces are hydrophilic. The results obtained here can be used to separate materials with different hydrophobicity and hydrophobicity properties.