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**Simulating Heat Flux and Bubble Nucleation using Molecular Dynamics**[1] TASSOS KARAYIANNIS, Brunel University, EDWARD SMITH, Imperial College London, KHELLIL SEFIANE, University of Edinburgh , OMAR MATAR, Imperial College London — Modelling the heat flux in multiphase flow situations must account for nucleation of bubbles, non-linear heat transfer coefficients, complex molecular interaction at the surface, detailed surface textures as well as build up of material on the surface. These complex factors combine to define the well known boiling curve, which characterises the heat flux for a given temperature gradient. Understanding and optimisation of this boiling curve, and its critical heat flux (CHF), is a problem of great importance. Molecular dynamics (MD), by modelling the motion of the individual molecules, can replicate the bubble nucleation and heat flux. Details of the wall-fluid interaction are represented with complex textures and the surface materials can be explicitly reproduced. In this talk, MD simulation results are presented for bubble nucleation and heat flux. The heat flux is matched to experimental results and the process of nucleation explored for both fractal and textured surfaces. The unique insights from the molecular scale are discussed and potential applications including surface design and coupled molecular to continuum simulation are presented.

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