Public Abstract

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Title:MICRO-SCALE HEAT TRANSFER SIMULATION ON WATER WITH MOLECULAR DYNAMICS AND HYBRID APPROACH

Water is most widely existing liquid in the earth; beyond all question, it takes a very important role in human daily life and many applications in industrial field. The heat transfer phenomena have drawn a great attention in the past decades. In the thesis, classical molecular dynamic simulations are carried out to study thermal and dynamic properties, including thermal conductivities, specific heat capacity, and shear viscosity. Though water molecule only has three charged atoms, but a number of water molecule models exist in the literature field. In this thesis, several rigid water molecule models are selected to perform the simulation. Then a non-equilibrium molecular dynamic is conducted to study nano-bubble growth and annihilation in the liquid water with rigid TIP3P. A nano-bubble is successfully generated, and pressure and surface tension of the bubble is obtained. Contact angle of a water droplet is also getting attention from micro- cooling engineers. A non-equilibrium molecular dynamics on contact angle of nano-size water droplet on a single wall carbon nanotube plate is performed. The gap distance between nano-tube affects the contact angle somehow, and a critical distance value that achieve largest contact angle is found. Rapid boiling phenomena of thin water film on a hot copper plate is also studied due to its application in various industrial fields, such as laser cleaning, thermal ink-jet printer, medical surgery. The entire process of the boiling phenomena is observed, and a piston-like motion of the film is analyzed. To the end, due to the size limitation of classical molecular dynamics, a hybrid simulation coupling molecular dynamic and computational fluid dynamic is developed to extend the simulation size to micron based on open-source code LIGGGHTS and OpenFOAM. Heat transfer coefficient between argon flow and cold copper plate is studied and it is found that heat transfer coefficient can reach a very high value. In the future work, argon fluid could be replaced with normal liquid water molecules, and some similar or more complicated simulation can be performed within current framework.