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Simulation of Water-Droplet Flows in a Straight Microchannel having a Sub-zero Temperature Wall Using Many-body Dissipative Particle Dynamics

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The transport phenomena with phase change at nano/micro scales have become a great topic of interest due to the development of nanotechnology. Nanotechnology has developed a number of engineering devices, such as the MEMS/NEMS devices and porous membranes in sustainable energy devices (e.g., fuel cells). The characteristic lengths of these components are micro, sub-micron and even nanometer scales and the transport phenomena indicate that the phenomena can no longer directly follow the conventional continuum assumptions. Therefore, it is significantly needed to fundamentally investigate the phenomena at such scales in various applications. This is the motivation of our study.

In this study, we focus on the dynamics and phase change phenomena of water in a parallel-plate microchannel under the sub-zero temperature condition. This study is numerically conducted by employing dissipative particle dynamics with an additional many-body term (MDPD) enabling the system to be multi-phase. This method is a coarse-grained version of molecular dynamics and has been widely used for a number of studies on nano/micro-scopic transport phenomena of fluids. Also, this method is combined with the energy conserving DPD (DPDe) in such a way that the simulation can capture energy transport and phase change as well as the dynamics of liquids. Thus, the methodology used in this study can be called MDPD with energy conservation (MDPDe).

This study starts from performing a set of benchmark simulations to validate the dynamic and thermal properties of water in the MDPDe method. The latent heat model is utilized to simulate the solidification/melting of water in this study. The simulations concern a water droplet flowing through a straight-channel having different constant temperatures at the top and bottom walls, where the temperature on the bottom wall is lower than the melting temperature. The results are shown in the form of the droplet shape for different wall wetting conditions and the effects of hydrophobic and hydrophilic walls on the flow characteristics and formed ice on the bottom wall are discussed.