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Numerical Study of Homogeneous Nanodroplet Growth

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Abstract : Drop condensation is the phenomenon that the tiny drops form when the oversaturated vapour present in the environment condenses on a substrate and makes the droplet growth. Recently, this subject has received much attention due to its applications in many fields such as thin film growth, heat transfer, recovery of atmospheric water and polymer templating. In literature, many papers investigated theoretically and experimentally in macro droplet growth with the size of millimeter scale of radius. However few papers about nanodroplet condensation are found in the literature especially theoretical work. In order to understand the droplet growth in nanoscale, we perform the numerical simulation work to study nanodroplet growth. We investigate and discuss the role of the droplet shape and monomer diffusion on drop growth and their effect on growth law. The effect of droplet shape is studied by doing parametric studies of contact angle and disjoining pressure magnitude. Besides, the effect of pinning and de-pinning behaviours is also studied. We investigate the axisymmetric homogeneous growth of 10–100 nm single water nanodroplet on a substrate surface. The main mechanism of droplet growth is attributed to the accumulation of laterally diffusing water monomers, formed by the absorption of water vapour in the environment onto the substrate. Under assumptions of quasi-steady thermodynamic equilibrium, the nanodroplet evolves according to the augmented Young–Laplace equation. Using continuum theory, we model the dynamics of nanodroplet growth including the coupled effects of disjoining pressure, contact angle and monomer diffusion with the assumption of constant flux of water monomers at the far field. The simulation result is validated by comparing with the published experimental result. For the case of nanodroplet growth with constant contact angle, our numerical results show that the initial droplet growth is transient by monomer diffusion. When the flux at the far field is small, at the beginning, the droplet grows by the diffusion of initially available water monomers on the substrate and after that by the flux at the far field. In the steady late growth rate of droplet radius and droplet height follow a power law of 1/3, which is unaffected by the substrate disjoining pressure and contact angle. However, it is found that the droplet grows faster in radial direction than high direction when disjoining pressure and contact angle increase. The simulation also shows the information of computational domain effect in the transient growth period. When the computational domain size is larger, the mass coming in the free substrate domain is higher. So the mass coming in the droplet is also higher. The droplet grows and reaches the steady state faster. For the case of pinning and de-pinning droplet growth, the simulation shows that the disjoining pressure does not affect the droplet radius growth law 1/3 in steady state. However the disjoining pressure modifies the growth rate of the droplet height, which then follows a power law of 1/4. We demonstrate how spatial depletion of monomers could lead to a growth arrest of the nanodroplet, as observed experimentally.

Keywords : augmented young-laplace equation, contact angle, disjoining pressure, nanodroplet growth
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