Title of Ph.D. thesis:

Instabilities in inhomogeneous/nanoparticle laden thin liquid films under different force fields

Name of the student: Manga Ramya Durga

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Abstract

This thesis studied the stability of different types of thin liquid films using various numerical techniques. First, we studied the stability of non-magnetic, inhomogeneous (viscosity decreases with a decrease in film thickness) thin liquid film between two solid substrates with an air gap using a continuum approach. Navier-Stokes (NS) equations are simplified in the continuum approach using lubrication approximation, resultant fourth-order partial differential equation discretized using second-order central finite difference scheme (FDM), and time-integrated using Gear's algorithm. The net force acting on the system is due to the van der Waals (vdW) attractive force between the free interface of film and the bottom substrate-film interface and the short-range attractive force between the film-free interface and top substrate. The decay length (l_p) determines the distance from the top substrate in which short-range force is effective. T. Kotni et al. reported sub-spinodal length scales under vdW force if the film's mean thickness (h_o) lies in the spinodal range and the spinodal range depends on the viscosity parameters $\left(M_1, r_g, p\right)$. Depending upon the top surface position (d) and decay length (l_p), film experiences a short-range force in different stages of dewetting. At very low values of d (> h_o) or at higher values of l_p, short-range force interferes with the bottom dewetting and forms a single hole in λ_{dom}. Whereas at lower values of l_p, the film experiences a short-range force in the hole growth face and forms more than one hole in λ_{dom}. At lower values of l_p, a maximum number of holes in λ_m will form when the strength of short-range force ($|S^{AB}| < |S^{LW}|$) is moderate, the position of the top surface is at $2h_o$, and when h_o is in spinodal range.

The lubrication approximation is not valid for all the types of liquid thin films. For example, in metallic films, contact angles are greater than 30^o, and inertial forces are also significant. So, there is a need to solve the NS equation without simplification. The second objective of the thesis

is to investigate the stability of homogeneous thin liquid films under vdW force by indirectly solving NS equations using one of the mesoscopic approaches, the Lattice Boltzmann method (LBM). The stability analysis is carried out using a single-component multiphase (SCMP) pseudopotential LBM with a multiple-time relaxation (MRT) time collision operator at the density ratio 98.48, in both 2D and 3D. D2Q9 and D3Q15 lattice models are used in 2D and 3D, respectively. In-house codes are developed using C language, and 3D LBM codes are parallelized using a message-passing interface (MPI). The reported dewetting stages, namely, the arrangement of fluctuations on a dominant wavelength, hole formation, and expansion, are successfully observed with the present numerical method in both dimensions. The breakup of liquid threads between the holes into droplets due to Rayleigh instability is also captured in 3D. In 2D, at the time of initial rupture of the film $\left(\lambda_{dom,rup}\right)_{avg}$ is calculated by DFT and observed $\left(\lambda_{dom,rup}\right)_{avg} > \lambda_{dom,LSA}$. The deviation of $\left(\lambda_{dom,rup}\right)_{avg}$ from $\lambda_{dom,LSA}$ is due to shear stresses at the interface, high contact angles, and diffused interface.

In the third objective, the stability of ferrofluid thin films under magnetic and vdW forces is studied. Ferrofluids are colloidal suspensions of magnetic nanoparticles of diameter less than 15 nm. The present work considered ferrofluid as a single-phase magnetizable liquid. Along with the NS equations, Maxwell's equations of magnetism also play a role in dictating the stability of ferrofluids. The resultant equation for magnetic potential obtained from Maxwell’s equation is discretized using a second-order central finite volume scheme (FVM). The resulting system of linear equations is solved using the alternating direction implicit method, and SCMP MRT LBM solves NS equations. The coupled algorithm of SCMP MRT LBM and FVM is known as hybrid LBM (HLBM) since two different numerical methods are used to solve NS and Maxwell equations. An in-house code was developed, and the stability of ferrofluid thin films under different magnetic field directions along with vdW force was studied. The instability of the interface depends on the nature of the vdW force, the direction of the external magnetic field, $Bo_m\left(=\frac{\mu_o\, h_o\, H_o^2}{2\gamma}\right)$, and $\frac{\mu_l}{\mu_v}$. If the ferrofluid completely wets the substrate under the horizontal magnetic field, the interface oscillates in the longitudinal direction when $Bo_m > Bo_{cri}$. Whereas under the vertical magnetic field, undulations grow into peaks. The number of peaks at the interface is a function of $Bo_m, \frac{\mu_l}{\mu_v}$, and h_o. Also, the drop is pinching under the vertical magnetic field due to Plateau instability. At high values of Bo_m and $\frac{\mu_l}{\mu_v}$, elongation of the drop increases, resulting in more than one daughter droplet, whereas at low values, the entire drop detaches from the substrate. The dewetting of the film is observed under both the horizontal and vertical magnetic fields when $A_{eff} > 0$. The number of drops depends on the strength of the vdW and magnetic forces. Due to a decrease in adhesive force, an entire drop detaches from the substrate.

The last objective investigated the stability of temperature-sensitive (TS) ferrofluids under a vertical magnetic field without vdW force. The NS and Maxwell equations are solved using HLBM, and the energy equation is discretized in space by FDM and time-integrated using the fourth-order RK method. The magnetization of ferrofluid is a linear function of an external magnetic field and temperature. For TS ferrofluids, the magnetic force is twice that of the temperature-insensitive ferrofluids. The physical properties of the ferrofluid and BF are independent of temperature except for density and surface tension. Because of the numerical method employed for the multiphase flow, surface tension is inherently a function of temperature. In the early stages, the deformation of the interface is only due to the magnetic force. The Marangoni flow also assists the peak formation because of the temperature variation along the interface as the interface deforms. The height and number of peaks for TS ferrofluid are more than those of the TIS ferrofluid film at a particular h_o and Bo_m. Also, the peaks are forming earlier than in the case of TIS films because of the increased magnetic force and Marangoni flow.