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ORIGINAL RESEARCH PAPER

Numerical Study of Bubble Separation and Motion Using Lattice Boltzmann Method

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ABSTRACT: In present paper acombination of three-dimensional isothermal and two-dimensional non-isothermal Lattice Boltzmann Method have been used to simulate the motion of bubble and effect of wetting properties of the surface on bubble separation. By combining these models, three-dimensional model has been used in two-dimension for decreasing the computational cost. Firstly, it has been ensured that the surface tension effect and Laplace law for two-density ratio 50 and 1000 have been properly implemented. Secondly, by simulation of static droplet in different conditions wettability, integrity applied equations has been investigated.Thirdly, effect of governing dimensionless numbers such as Etvos number and Morton number on Reynolds number and terminal shape of bubble have been investigated.Different flow patterns in various dimensionless numbers have been obtained and by changing the dimensionless number, terminal change of bubble's shape has been seen. Finally, the impact of wettability of surface on departure of bubble from wall under buoyancy force in different dimensionless numbers has been studied.

KEYWORDS: *Etvos Number; Inamuro Model; Lattice Boltzmann Method; Morton Number; Two Phase Flow; Wettability*

INTRODUCTION

In scientific point, many phenomena in daily life are two-phase or multiphase, for example, the raindrops motion; dust particles motion in the air or the wave motion on the sea surface, and its failure modes are examples of two-phase issuesoccurs in nature. Two-phase fluid with many application uses in industrial issues, for example, uses in boilers. In boilers, combination of water and vapor as a two-phase fluid has an important role in boiler design.

In addition,two-phase fluid with main application is used in nuclear reactor design. As well as designing advanced tools like rocket engines, water purifier and blood pumping machines needdetailed knowledge in dynamic of multi-phase flow. Checking the bubble motion in fluids in many applicationsis used in petroleum and chemical industries and it is because of the mixture of gas and liquid broadly in these industries.The physical mechanism of two-phase flow is very complex. Thus, clear perception of two-phase flow mechanisms is not available. The numerical investigation in two-phase flows is significant due to disability of experimental investigations to access to the physical parameters in the bubble and droplet. Thus, numerical investigation is preferable for this phenomenon. The lattice Boltzmann method is almost new numerical techniques based on kinetic theory, whichis used for investigation of fluid flows.In Comparison with the traditional CFD, LBM has some advantages such as easy process, simple and efficient implementation for parallel computation, simple and efficient implementation for parallel computation, simple and strong handling of complex geometries, etc. There are various versions, which provided for two-phase flows using Lattice Boltzmann method.

Gunstensen et al [1] presented a multi component model based on two dimensional lattice-gas hydrodynamics. In their model two-particle distribution functions, red and blue, were introduced for studying two different fluids. Shan and Chen [2] offered a method for multicomponent and multiphase flows with regard microscopic interaction. Swift et al [3] proposed a model for multiphase and multicomponent flows by using free energy approach. The main advantage of this model is the ability to include multi component and non-ideal thermodynamics of fluid in isothermal.

It is worth mentioning that, in the all listed LBM two-phase models, the density ratio is intended less than 10, while in fact density ratio is more than 10 at most of the liquid-gas systems. Main problem in numerical solution of two-phase flow with large density ratio is numerical instability in interface.

Inamuro et al [4] offered a new model based on free energy approach for two-phase flow with high density ratio and investigated motion of a single bubble and many bubbles under buoyancy force in three dimensions(3D) simulation. Inamuro et al [5] used their method to study rising of two droplet and their coalescence in a vertical and horizontal rectangular channel.

In another study, Inamuro et al [6] employed this model to simulate coalescence of two droplet with equal diameter with initial velocity in 3D and also two droplet with unequal

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Nomenclature

		E	Etvos number
f_i^c	specific heat ($Jkg^{-1}K^{-1}$)		**Greek Symbols**
g_i^c	diameter (nm)	Δx	spacing of square lattice
d	grashof number	Δt	time step in the scale of LBM
h_i^c	gravitational acceleration ($m.s^{-2}$)	μ	dynamic viscosity ($kgm^{-2}s^{-1}$)
g	height of the enclosure (m)	v	kinematic viscosity (m^2s^{-1})
H	thermal conductivity ($Wm^{-1}K^{-1}$)	θ	Contact angle
c_i	Nusselt number	ρ	density(kgm^{-3})
E_i	pressure ($kg\ m^{-1}s^{-2}$)	ρ_l	Density of liquid
p	dimensionless pressure	ρ_g	Density of gas
f_i	Rayleigh number	ζ	direction normal
g_i	Richardson number	σ	interfacial tension
h_i	Reynolds number		**Subscripts**
Re	Prandtl number	α	coordinate
k_f	temperature (K)	β	coordinate
P_0	dimensional x and y components of velocity	i	Particle Counters
u, v	dimensionless velocities	f	fluid
U,V	reference velocity	l	liquid
M	dimensional coordinates	g	gas
x, y	dimensionless coordinate	0	reference

diameter in 3D [7]. Inamuro [8] carried out simulation of a set of bubbles in a branch channel, this geometry was utilized as a cooling system in air conditioning system. Yan and Zu [9] simulated horizontal movement of two bubbles with initial velocity in 3D channel. Yoshino and Mizutani [10] studied contact angel by adding thewettability condition to Inamuro[4] method. Yan and Zu[11]investigated the final shape of droplet on surface in different wettability and also they studied the final shape of droplet on partial wetting surface in 3D. in [12] Yan and Zu studied rising two bubbles, their coalescence and shape of droplet on partial wetting surface. Later on making some changes on the original model was used by Tanaka [13-14] for two dimensional and reactive flows. Tanaka et al.[13] simulated dynamic treatment of droplet on solid surface. Moreover, they used this model for investigation of boiling process[14]. Sattari et al. [15] by combining Tanaka [13] and Inamuro's model [4], investigated nucleate pool boiling and transient boiling in 2D.

In addition to Inamuro[4], Lee and others have presented their proposed method in two-phase fluid flows with high density difference[16-19]. One of the technologies that are now widely used in the industries of textile, automobile, light industry, shipbuilding and aviation has many applications, are self-cleaning surfaces. Based on several studies, high hydrophilic and hydrophobic surfaces have this type of property.

This phenomenon occurs as a droplet place on these surfaces.Although the effect of contact angle on a droplet on the surface and its evaporation have been studied[9-13, 17, 18].

In this paper, for the first time the effect of the surface wetting properties on the motion of bubble, in the case of washing machines with steam mechanismis studied. Inamuro model[4] is a 3D model so has high computational cost, Tanaka [14]added derivative of pressure tensor term to Inamuro[4] model for simulation of boiling in two dimensions and it increases computational cost in twodimensions.

In this study, firsta combined model is presented by implementation of Inamuro[4] and Tanaka[14]methods. After that, this model was used to ensure the proper functioning of the effect of surface tension. For this purpose, two testshave been conducted: the first test was related to a two dimensional square bubble,placed in a liquid.

In the second test, two circular bubbles have been placed side by side and their approach was modeled. After that the Laplace law has been checked, and then the effect sof dimensionless numbers for a bubble rising by bouncy force have been investigated. Endmost rising of bubble have been modeledfrom surfaces with different wet properties in different dimensionless numbers.

Methodology

In the present paper, the combined method that has been introduced in pervious study [15], is employed for 2D simulation. In this paper, three distribution functions have been used. f_i, g_i and h_i to calculate order parameter which distinguishes two phases, a predicted velocity and pressure, respectively.

$$f_i(x + c_i\Delta x, t + \Delta t) = f_i^c(x,t) \tag{1}$$

$$g_i(x + c_i\Delta x, t + \Delta t) = g_i^c(x,t) \tag{2}$$

$$h_i^{n+1}(x + c_i\Delta x) = h_i^n(x) - \frac{1}{\tau_h}\left[h_i^n(x) - h_i^c(x)\right] - \frac{1}{3}E_i\frac{\partial u_\alpha^*}{\partial x_\alpha}\Delta x \quad (3)$$

f_i^c, g_i^c and h_i^c are equilibrium distribution functions. ΔX is spacing of square lattice and Δt is time step in the scale of LBM during which particles travel in lattice spacing. Equilibrium distribution functions in equation (1-3) are obtained by following equations:

$$f_i^c = H_i\phi + F_i\left[p_0 - k_f\phi\frac{\partial^2\phi}{\partial x_\alpha}\right] + 3E_i\phi c_{i\alpha}u_\alpha + E_i k_f G_{\alpha\beta}(\phi)c_{i\alpha}c_{i\beta} \quad (4)$$

$$g_i^c = E_i\left[1 + 3c_{i\alpha}u_\alpha - \frac{3}{2}u_\alpha u_\alpha + \frac{9}{2}c_{i\alpha}c_{i\beta}u_\alpha u_\beta\right] + E_i + \frac{3}{4}\Delta x\left(\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial u_\beta}\right)c_{i\alpha}c_{i\beta} - 3E_i c_{iy}\left(1 - \frac{\rho_G}{\rho}\right)g\Delta x + E_i\left[3c_{i\alpha}\frac{\Delta x}{\rho}\frac{\partial}{\partial x_\beta}\left\{\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta}\right\}\right] + E_i\frac{k_g}{\rho}G_{\alpha\beta}(\rho)c_{i\alpha}c_{i\beta} - \frac{1}{2}F_i\frac{k_g}{\rho}\left(\frac{\partial\rho}{\partial x_\alpha}\right)^2 \quad (5)$$

$$h_i^c = E_i P^n(x) \quad (6)$$

For reading more detailed, see our pervious study [15].

Wetting boundary condition

When gas and liquid interface placedon a solid wall, a finite constant contact angle is indicated as wettability of system, which is caused by balance of surface tension forces. To apply these conditions, Yoshino's model[10] which is resulted from combining methods of Briant [20] and Inamuro [4], is employed. In this model, the finite-difference of the order parameter on the boundary is obtainedby:

$$\left.\frac{\partial^2\phi}{\partial\xi^2}\right|_{\xi=0} \approx \frac{1}{2}\left(-3\left.\frac{\partial\phi}{\partial\xi}\right|_{\xi=0} + 4\left.\frac{\partial\phi}{\partial\xi}\right|_{\xi=1} - \left.\frac{\partial\phi}{\partial\xi}\right|_{\xi=2}\right) \quad (7)$$

where, ζ is the direction normal to the wall. In this correlation, the first term on the right hand side is attained by a forward finite-difference scheme; the second term is calculated by a standard centered finite-difference scheme. In addition, the third term is obtained by a backward finite-difference scheme, to wit:

$$\left.\frac{\partial\phi}{\partial\xi}\right|_{z=2} \approx \frac{1}{2}\left(3\phi\big|_{\xi=2} - 4\phi\big|_{\xi=1} + \phi\big|_{\xi=0}\right). \quad (8)$$

RESULTS

Validation of two phase solution

Since the most important and sophisticated part of an analysis oftwo-phase flow is related to dynamic interface between two fluids, first step for the demonstrating accuracy of the flow simulation is checking this issue. Two tests werecarried out for this issue. In the first test, deformation of a two dimensional square bubble that has been placed in filled environment of liquid has been shown. According to effects of surface tension between two fluids, the bubble tends to change to steady state with the lowest interface. According to simulation results shown in Figure 1, bubble shape has changed by passing the time and became like a circle. This issue shows the effects of surface tension, which are important part of two-phase flow analysis, are properly. This test has used as a credit of two-phase solution by Mousavi et al. [21] . This test has been done for large density ratio(1000). As Inamuro in [4]mentioned, increasing of density ratio leads to increasing the iterationnumbers to achievedesired results.As Figure 2 shows, deformation occurred in moreiterations.

For a static bubble, the velocity must be zero at all points in equilibrium condition. However, in two-phase numerical methods, a spurious nonphysical velocity is created around the bubble near the interface. Indeed today, the numerical methods are improving for decreasing this spurious velocity [22]. Because of this spurious non-physical velocity in numerical methods, weak vortices are created around the droplet and bubble, near interface these velocitieshave been called parasitic flow. Figure 3 shows parasitic flows around a bubble in an equilibrium condition in one of the performed simulations. In second test, two circular bubbles with same diameter *L/3* have been located adjacent to each other. In this simulationthe distance between two bubbles, density and viscosity are equal to 0/05, 1 and 0.01, respectively. Due to effects of surface tension and Van der Waals forces, these bubbles approach and finally a circular larger bubble is created. The results of this simulation have been shown in Figures (4-5). This test has been used as a credit of two phases solution[19, 21].

Laplace law

Laplace law represents the correlation between inner P_{in} and outer pressure P_{out} of bubble with interfacial tension σ between two fluids. Based on Laplace law there is a formula for a two dimensional bubble[1]:

$$P_{in} - P_{out} = \frac{\sigma}{R} \quad (9)$$

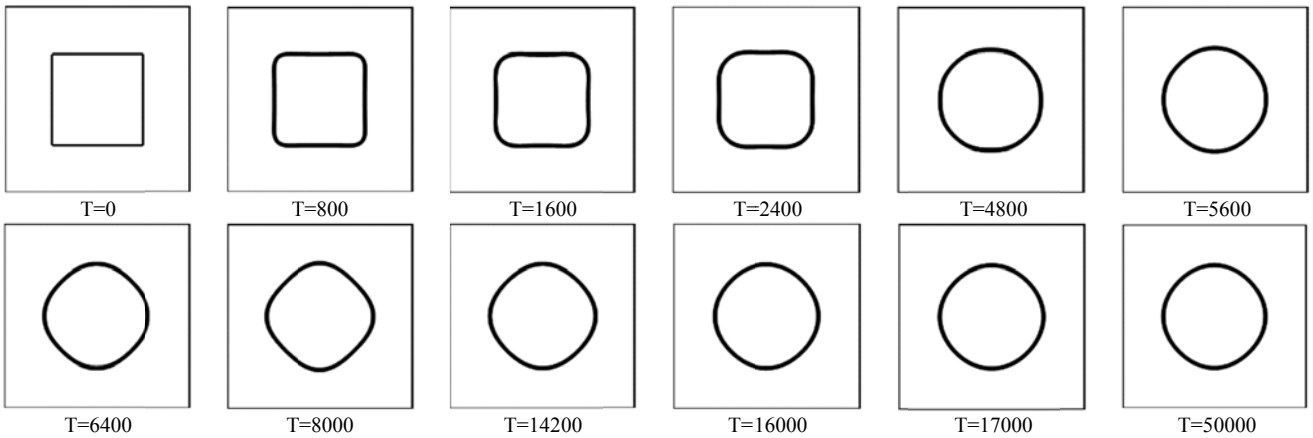


Fig. 1. a square droplet deformation at lattice time steps for density difference 50

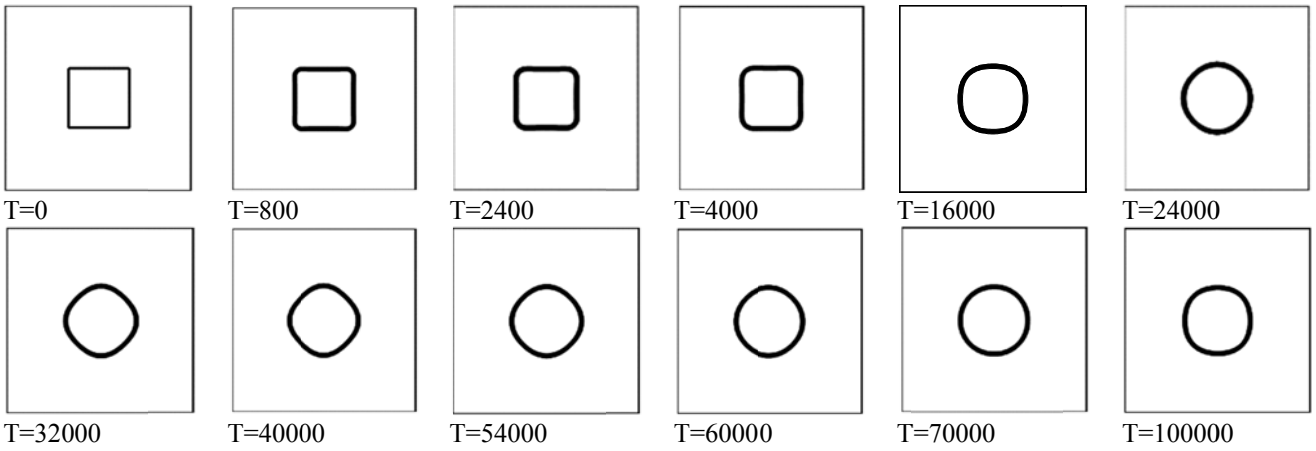


Fig. 2. a square droplet deformation at lattice time steps for density difference 1000

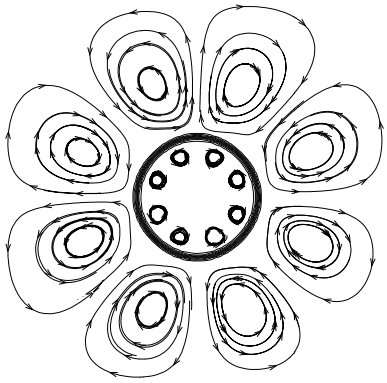


Fig. 3. the parasitic flow around a bubble

Surface tension during the compressibility and isothermal flows is one of the constant properties of two fluids.

Therefore, it can be concluded that a linear relationship exists between the pressure difference between the inside and outside the bubble with the inverse radius in the same conditions without changing its properties.

Figure 6 shows the performed simulation and obtained pressure has been satisfied nicely the Laplace law in Lattice Boltzmann Method. This test has been done as credit of two-phase solution in [1, 3, 19, 21] .

Independence of mesh

To do this, two different tests have been performed. In the first test, Laplace law has been performed for various grids and note that the related slop is equal to surface tension so the values have been obtained and compared in different grids. In second test, three different grids

200×100, 100×50, 300×150 have been used and the bubble final regimes have been compared. The results of the first test have been shown in Figure 7 and Table 1, due to these results, suggested grid number is 100 for length of the domain, because of the equality of surface tension force in 100×100 and 120×120 grids.

The results of second test have been shown in Table 2; the final shape of the bubble is not true in grid 50×100 by changing of dimensionless numbers in comparison with previous works. However, the final shapes of the bubble and flow regimes in 200×100,300×200 grids are completely equal. In this paper 200×100 grid have been used in order to avoid increasing the computational cost.

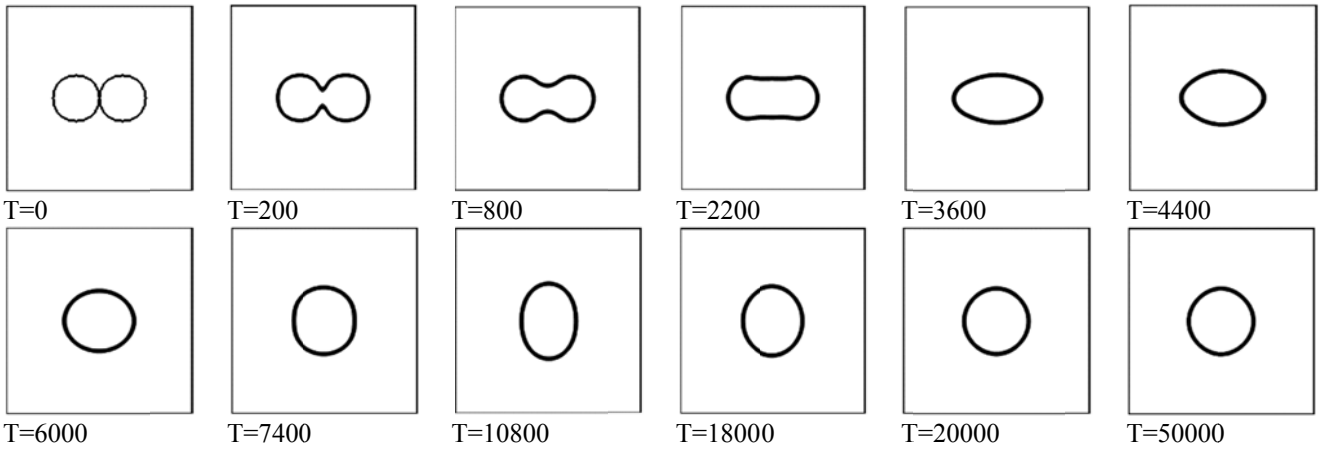


Fig. 4. Coalescence of two bubbles in density ratio 50

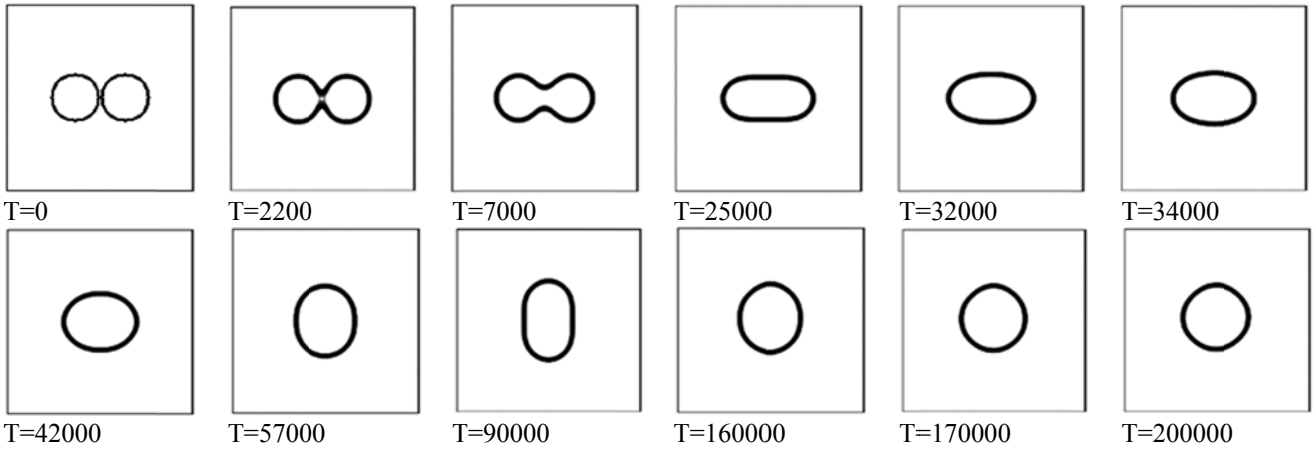


Fig. 5. Coalescence of two bubbles in density ratio 1000

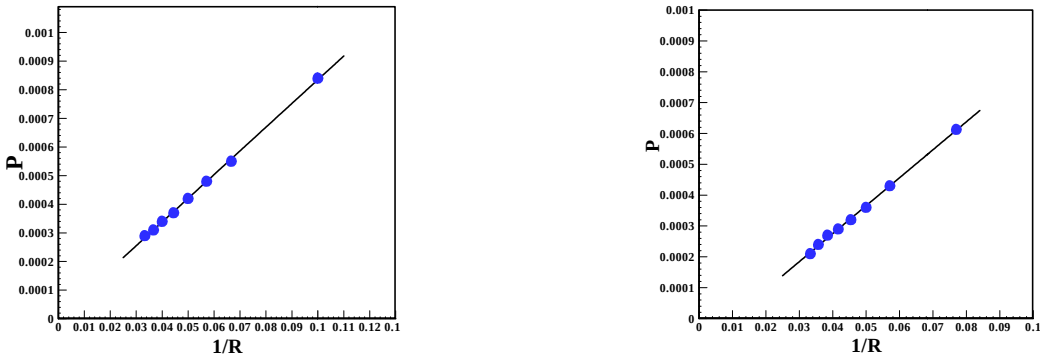


Fig. 6. simulation for Laplace law (a) density ratio 50 and (b) density ratio 1000

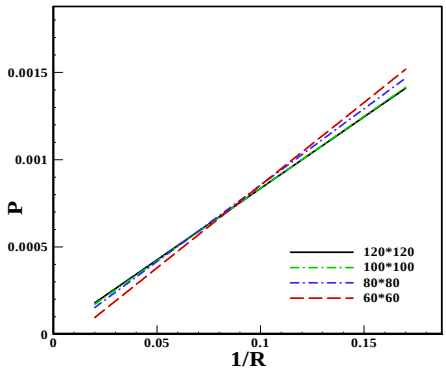


Fig. 7. Laplace low in different grid

Table 1
The surface tension force in lattice unit In different grids.

mesh	60×60	80×80	100×100	120×120
Surface tension	0.0094	0.0088	0.0082	0.0081

Table 2
flow regime in different dimensionless numbers.

Dimensionless numbers	**50×100**	**100×200**	**150×300**
E=1, M=0.001	spherical	spherical	spherical
E=5, M=0.001	spherical	ellipsoidal	ellipsoidal
E=116, M=266	spherical	ellipsoidal cap	ellipsoidal cap
E=20, M=0.0001	ellipsoidal	disc	disc
E=42, M=0.001	ellipsoidal cap	spherical cap	spherical cap
E=339, M=43	skirt	skirt	skirt

Rising bubble

In this section, the bubble motion in a fluid-filled environment has been investigated. The dimensionless numbers of this phenomenon are Morton($M=gul(\rho_l-\rho_G)/\rho_l^2\sigma^3$), Etvos ($Eo=g(\rho_L-\rho_G)D^2/\sigma$) and Reynolds numbers ($Re=\rho_L DV/\mu L$) which V is final velocity of the bubble and D is the initial diameter of the bubble.

The opposite boundaries have the periodic boundary conditions. The grid 100×200 has been used. The initial diameter of the bubble has been 30-lattice unit.

Behavior comparison of bubble in two dimensions has been indicated that bubble deformation is a function of Etvos and Morton numbers [4] . According to the terminal shape of bubble which are different in different dimensionless numbers, various patterns of flow in two-phase flow are divided to six major groups are shown in Figure 8 : 1)spherical, 2)ellipsoidal, 3)ellipsoidal cap, 4)disk, 5)spherical cap, 6)skirt [4] . The results have been represented in dimensionless time $T=t/t_n$ with $t_n=\sqrt{d/g}$ where t is number of iteration. When the bubble moves upward, at first, the bubble starts to move due to density difference with the surrounding fluid leads to buoyancy force.

The Drag force on the bubble is because of the bubble motion in the fluid and if the bubble does not burst, will reach to the constant velocity and shape. In this mode, buoyancy force is equal to fluid drag force and the bubble continues to move with the same constant velocity.

In Figure 8 in right column, density linear contour with velocity vectorshave been drawn for related dimensionless numbers when the shape of bubble is stable and in left column, movement and shape of the bubble have been drawn in different dimensionless times. As seen in Figure 8, the shape of the bubble is the same for each of the regimes in last dimensionless times due to equivalence between buoyancy and drag force and stable bubble. Of course, the flow is unstable in Figure 8f and the bubble bursts and some parts of it separate after T=5 as shown in Figure 8.f. As seen in Figure 8, bubble deformation is such as concavity in the bottom of the bubble. In the lower part of the bubble, it should balance itself with the pressure inside of the bubble, because of the hydraulic pressure so convexity in liquid and concavity inside the bubble has been formed.

The higher pressure difference creates the larger vortex around the bubble and as a result, deformation of bubble is more. In Figure 8a almost the mentioned area has not been formed so the shape of bubble is stable. From Figure 8b onward have been increased size this area so bubble deformation have been increased. Figure 8a bubble deformation is not large but as is evident from the definition of dimensionless numbers, with the increasing of Etvos number as shown in Figures (8-a) and (8-b) buoyancy

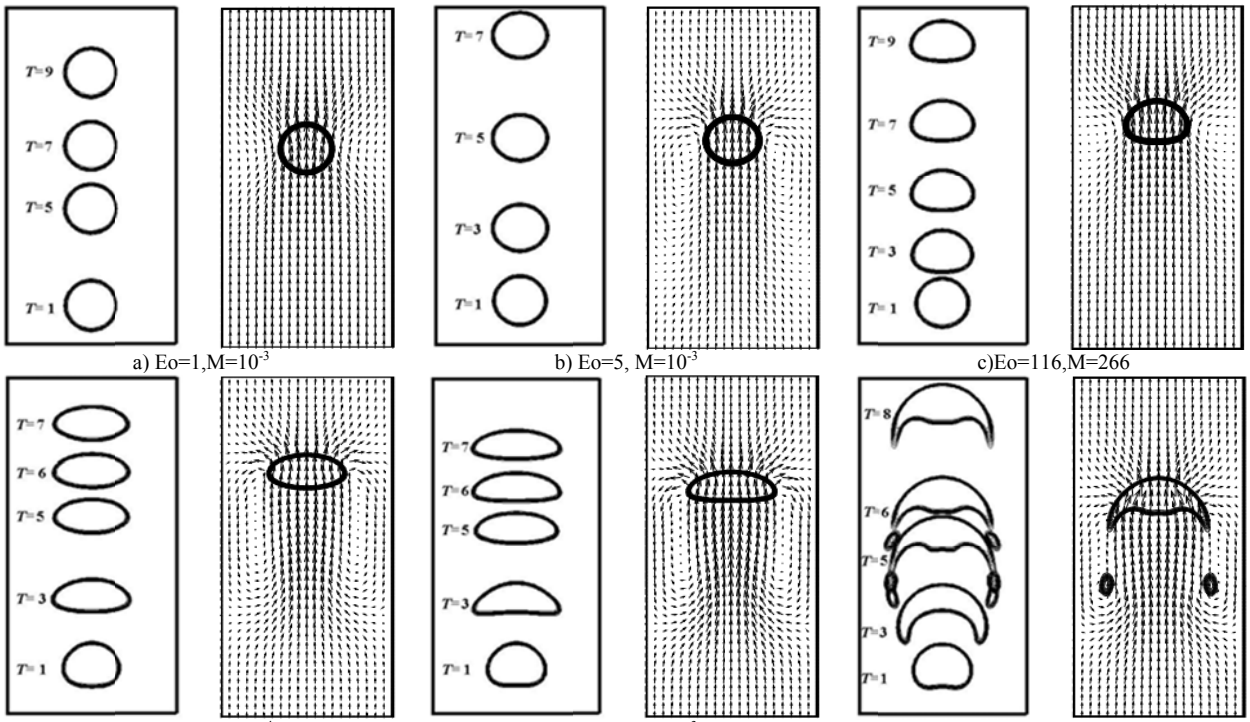
force has been increased and thus deformation of bubble is more. Also the surface tension decreases by increasing Etvos number because the surface tension is resistance to deformation, in other hand, increasing of Etvos number causes the increasing of deformation, increasing of Morton number causes increasing of bubble deformation but have less effect on bubble deformation because the Morton number connects with the surface tension in power 1/3 as seen on Figures 8(d-e).

According to different dimensionless times in Figure 8, it has been shown by changing dimensionless numbers, required time for passing the length of the channel has been changed and this represents the change in velocity and terminal Reynolds.

In Table 3, the terminal Reynolds number values have been calculated.

In Figure 9, streamlines for these bubbles have been plotted. In the first three cases, vortices have been formed only inside the bubble but after Figure (9-d) vortices have been formed under the bubble that called bubble trail. Bubble trail leads to turbulent flow around the bubble.

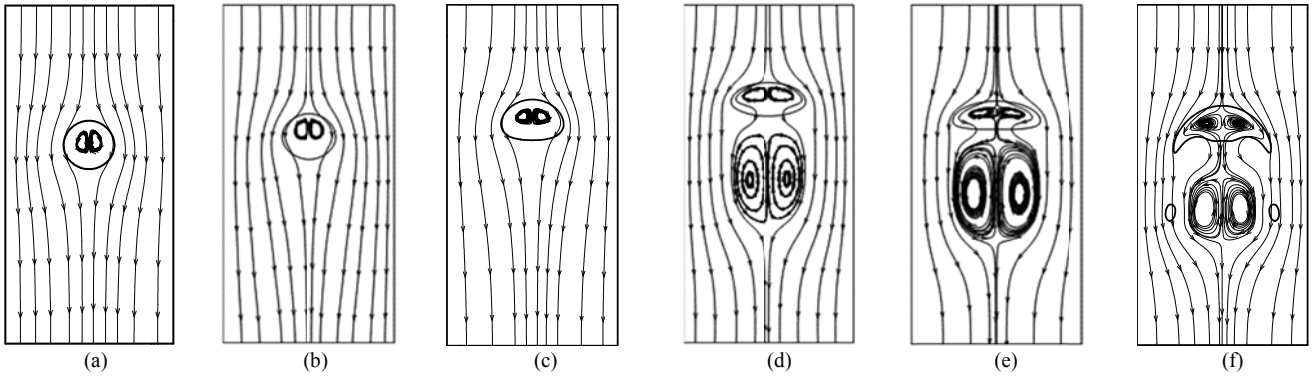
In the Figure 10, the obtained results are in good agreement in compared to Inamuro's three dimensional study [4] .



a) Eo=1,M=10^{-3} b) Eo=5, M=10^{-3} c)Eo=116,M=266

d)Eo=20,M=10^{-4} e)Eo=42,M=10^{-3} f) Eo=43,M=339

Fig. 8. Different flow regime in different dimensionless numbers



(a) (b) (c) (d) (e) (f)

Fig. 9. streamlines at different dimensionless number

Contact angles

For validation of wall boundary condition, a droplet placed on bottom wall with respect to properties of the surface. Simulated droplet contact angle with the wall surface, Figure 11, can be calculated by measuring the base and the height of the droplet.

If the base and the height of droplet define by H and L, respectivelythe droplet radius is obtained by using the following equation (Figure 11) [23] :

$$R = \frac{(4H^2 + L^2)}{8H} \tag{11}$$

The measured contact angle in the simulation is calculated from the following equation[23]:

$$\theta = \arctan\left(\frac{L}{2(R-H)}\right) \tag{12}$$

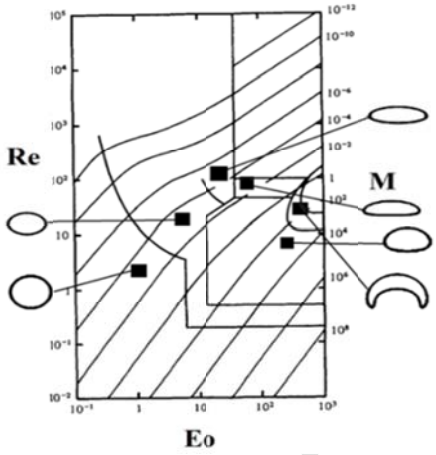


Fig.10. comparison of result of this study,■, and Inamaru's three dimensional study [4]

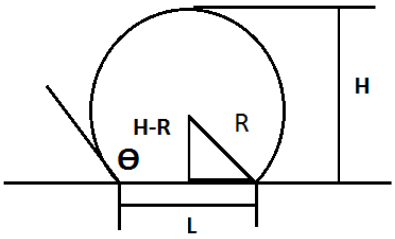


Fig. 11. Displaythe contact angle,Baseandheightdrops [23]

Table 3
Calculated Reynolds number corresponds to the different states of Figure 1.

1-1	1-2	1-3	1-4	1-5	1-6
4.62	21.95	7.63	105.08	93.47	34.84

As it is noted in[99], due to the fact that in this method,is calculatedregions with density gradient. For uniformity of results, boundary density has been considered $\rho=\rho_l+\rho_g/2$ at the separating boundary of two fluids. Figure 12 illustrates a droplet with initial diameter 40 grid units in a square enclosure with a length of 200 grid units. In Table 4,were compared desired contact angle values and obtained contact angles values from the simulations.As it can be seen, there is very little difference between these two values andthis negligible amount of error is acceptable.

Table 4
compares the desirable values of the contact angle and The contact angles obtained from the simulation

Desirable values of angles	Angle values obtained from the simulation
30	30.84
60	59.7037
120	119.931
150	150.341

Effect of wettability of surface on bubble separation

The simulations have been carried out for described regimes above in 5 different wettability.

Table 5
summarized results of simulation of effect of contact angles on bubble separation from wall.

Dimensionless number	Contact angles	Separation of surface	Become two pieces	Contact line
a)Eo=1,M=10^{-3}	30	✓	×	×
	60	×	×	×
	90	×	×	×
	120	×	×	×
	150	×	×	×
b)Eo=5,M=10^{-3}	30	✓	×	×
	60	×	×	×
	90	×	×	×
	120	×	×	×
	150	×	×	×
c)Eo=116,M=266	30	✓	×	×
	60	✓	×	×
	90	✓	✓	8.962
	120	✓	✓	18.281
	150	✓	✓	29.609
d)Eo=20,M=10^{-4}	30	✓	×	×
	60	✓	×	×
	90	✓	✓	8.626
	120	✓	✓	16.94
	150	✓	✓	27.384
e)Eo=42,M=10^{-3}	30	✓	×	×
	60	✓	×	×
	90	✓	✓	8.536
	120	✓	✓	15.906
	150	✓	✓	25.002
f)Eo=43,M=339	30	✓	×	×
	60	✓	×	×
	90	✓	✓	6.9774
	120	✓	✓	12.306
	150	✓	✓	16.2419

highly hydrophilic (30°), hydrophilic(60°), neutral(90°), hydrophobic(120°) and highly hydrophobic (150°). The results have been summarized in Table 5.

In addition, the examples of simulations have been given in Figure 13. In cases where, bubble cannot be separated from the surface, the final shape of bubble is in contrast to the final shape of the droplet in the same state. i. e. in angle of 30 degrees, which surface is hydrophilic, the final shape of the bubble is similar to the final shape of the droplet in hydrophobic conditions (i. e. angle 150 degrees). The surface that for a droplet is hydrophilic and the droplet tends to stick it when a bubble has been placed on it, the bubble tends to separate from it and vice versa. Separation occurs for Figures 13(a-b) only in the mode of highly hydrophilic,bubble detaches from the surface and in the other cases, by increasing Etvos numberdue to the high buoyancy force and overcomes the surface adhesion. Finally, the bubble detaches from the surface but it become to two pieces and some of it remains on the surface. Area of attached bubble to the wall with increasing contact angle increases. As seen from the Figure 13, due to similar terminal shape of bubble with obtained results in pervious section, itcan be concluded that terminal shape of the bubble is independent of surface properties.

According to Table 5, remained surfaceof bubble on the wall by increasing gravity force increases and in equal angles Figure 13f has lowest of it and in each group by increasing contact angles increases it**.**

Conclusion

In this paper, Inamuro's modelhas been used in two-dimensional coordination by combining the two-dimensional Tanaka's model and three-dimensional Inamuro's model. This method can be safely used to high density ratio of about 1000 in two dimensional due to the results tests of a square bubble in an environment which filled with liquid were valid and putting together the two bubbles and Laplace law for density ratio 50,10000. By comparing the results, changing in dimensionless numbers causes changing in gravity and surface tension. So different flow regimes occur and Etvos number have a greater impact on the flow regime than the Morton number. Different wettability condition of surface for a placed droplet on surface investigated and results show very good accuracy in obtained contact angles. Investigation of effect wettability of surface on bubble separation shows terminal shape of bubble is independent of properties of surface. By increasing Etvos number probability of bubble separation increases and length of line contact decreases. By increasing contact angles in equal dimensionless number length of line contact increases.

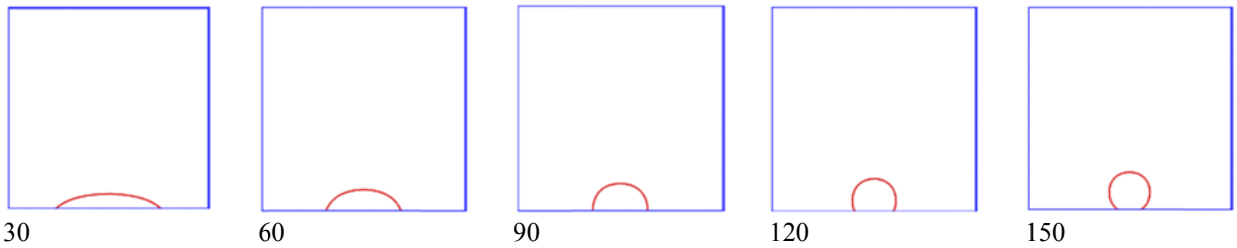


Fig. 12. Simulation of contact angles

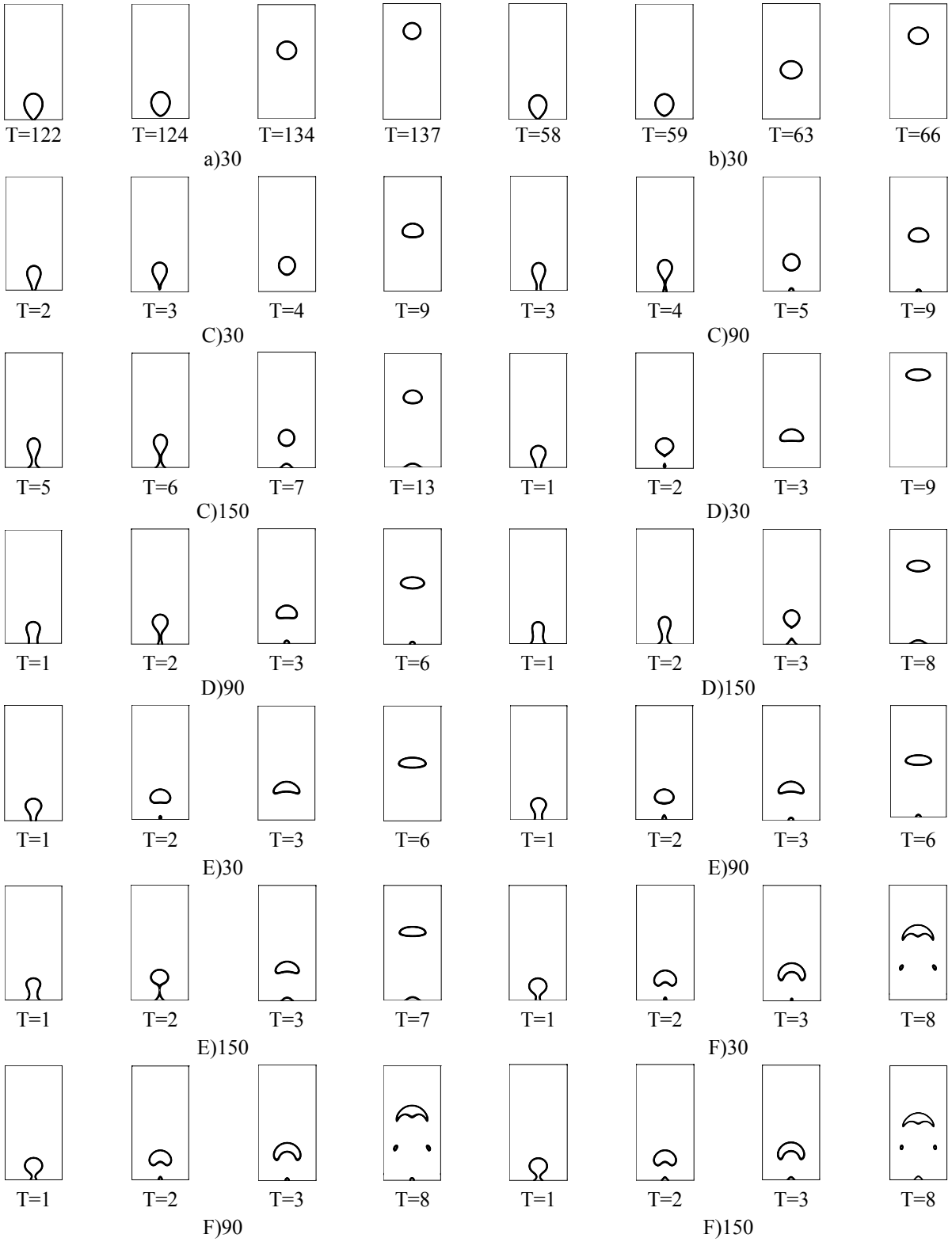


Fig. 13. Effect of wettability of surface on separation of bubble

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