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Re: SPE Paper #84892
Estimation of Surface Tension for Two Immiscible Fluids Using Lattice-Gas Automata

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SPE Paper 84892

Estimation of Surface Tension for Two Immiscible Fluids Using Lattice-Gas Automata

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This paper was prepared for presentation at the SPE International Improved Oil Recovery Conference in Asia Pacific held in Kuala Lumpur, Malaysia, 20–21 October 2003.

Abstract

Surface tension is one of the important properties in enhanced oil recovery, particularly for gas-liquid displacement in porous media and separation process. It acts to keep interfaces of two immiscible fluids smooth, where two or more curved interfaces create pressure differences. The estimation and measurement of surface tension currently are made by capillary rise such as the ring method and the pendant drop method. In this paper, the lattice-gas automata method is being explored to be used in estimating the surface tension between two immiscible fluids in a porous medium. The main idea of immiscible lattice-gas model in this paper was the introduction of two species of particles (red for gas and blue for oil) to represent two immiscible fluids. The great advantage of the model was that interfaces and the interfacial dynamics were generated spontaneously. The surface tension was estimated by the Laplace's equation and ranged between 0.00585 - 0.00603. In general, simulation results are in good quantitative estimation and this simulation also allow us to model liquid-liquid or gas-liquid interactions. The aim was to see the suitability of lattice-gas automata in representing two immiscible fluids of oil and gas.

Introduction

When two immiscible fluids, a liquid and a gas, are in contact with each other, they are in general separate by a thin layer called the interface, inter phase, or surface phase. From a mechanical standpoint, the system behaves as if it consisted of two homogeneous fluids separated by a uniformly stretched membrane.

The lattice-gas model of two-phase immiscible fluids was first proposed by Rothman and Keller (1988), based on the Frisch, Hasslacher, and Pomeau (FHP models, 1986). The models were later called Immiscible Lattice-gas (ILG) model. Their model has become an important tool for simulating the hydrodynamic of multiphase flow. In the Rothman and Keller model, the masses of the immiscible fluids species and the total momentum conserved locally and the choice of collision outcomes of each site depends on the color of the neighboring sites. In 1991, Somers and Rem introduced a local lattice-gas model for two-phase flow, which made the implementation on parallel machines faster and simpler. The basis of those two models was to let colored particles move along the direction of a local total color flux, and preserve the main properties of two-phase fluids. The evolution of the system on time-step to the next takes place in two successive stages, i.e., Propagation, the particles move from their node to the nearest neighbor in the direction of their velocity vector, and Collision, where every particle will change the arrangement of its configuration.

In this paper, a lattice-gas automata model was developed for simulating two-phase fluids (immiscible fluids) in a porous media. The lattice-gas automata model was extended to include interfaces between two fluids.

Surface Tension

Surface tension is defined as a force per unit length or energy per unit area. With reference to a bubble or a drop, we can consider a spherical cap as shown in **Fig. 1**, which is subjected to a surface tension (σ) around the base of the cap and to normal pressures P' and P'' at each point on the surface. As is evident from this figure, the effect of the surface tension (σ) is to reduce the size of the sphere unless it is opposed by a sufficiently great difference between pressures P'' and P'.

The surface is said to be in a state of uniform tension if: (a) at each point the surface tension is perpendicular to the dividing line and has the same value whatever the direction of this line, and (b) surface tension has the same value at all points on the surface. In this case, can be called the surface (or interfacial) tension of the surface: it has the dimension of force per unit length. From mechanical equilibrium of the surface, surface tension is expressed by the Laplace's equation, (Dullien, 1979)

$$P''-P'=\frac{2\sigma}{r} \qquad (1)$$

From Laplace's equation its shows that because of the existence of surface tension (σ) an arbitrary mean radius of curvature (r) maintains mechanical equilibrium between two fluids at different pressures P'' and P'.

Immiscible Lattice-Gas

In 1988, Rothman and Keller found that in the immiscible lattice-gas (ILG) model, color still moved with the flow but it also influenced where the flow goes. Specifically, the way in which collisions scatter momentum depended on the distribution of color at neighboring lattice sites. **Fig. 2**, illustrates the ILG microdynamics, the initial condition (a), the propagation step (b), and collision step (c). In the initial condition and propagation step, the particles propagate to the neighboring site in the direction of their velocity, where in the ILG some particles are red (bold arrows) while others are blue (double arrows). In the collision step, the collision rules change the configuration of particles so that, as much as possible, red particles are directed towards neighbors containing red particles, and blue particles are directed towards neighbors containing blue particles. The total mass, the total momentum, and the number of red or blue particle are conserved.

The colored state of the two-dimensional immiscible lattice-gas defined as follows, (Rothman, D *et al.* 1997),

$$s = (r, b) = (r_0, b_0, ..., r_6, b_6) \tag{2}$$

here the subscript with indices 0 represent rest particles, which increased the choice of collisions. The subscript with 1-6 indices refer once again to the lattice directions (unit velocity) c_i given by equation

$$c_i = \left(\frac{\cos \pi i}{3}, \frac{\sin \pi i}{3} \right), \quad i = 1, 2, ..., 6. \tag{3}$$

At most one particle of either color is allowed to move with a given velocity, and have

$$n_i = r_i + b_i \tag{4}$$

to indicate the presence of either a red or blue particle moving with velocity c_i, $i > 0$, or at rest ($i = 0$). The microdynamical equations for immiscible fluids given by

$$r_i(x + c_i, t + 1) = r_i'(x, t) \tag{5}$$

$$b_i(x + c_i, t + 1) = b_i'(x, t) \tag{6}$$

The post-collision states *r'* and *b'* depend on the configurations at neighboring sites. Specifically, the post-collision states are chosen with equal probability among the configurations *r'* and *b'*, where the color flux is,

$$q[r(x), b(x)] = \sum_{i=1}^{6} c_i [r_i(x) - b_i(x)] \tag{7}$$

and the color gradient or color field given by equation,

$$f(x) = \sum_i c_i \sum_j [r_j(x + c_i) - b_j(x + c_i)] \tag{8}$$

The set of post-collision states conserve colored mass and colored momentum, i.e.,

$$\sum_i r_i' = \sum_i r_i \qquad \sum_i b_i' = \sum_i b_i \tag{9}$$

$$\sum_i c_i (r_i' + b_i') = \sum_i c_i (r_i + b_i) \tag{10}$$

Model of Two-Phase Immiscible Fluids

In 1986, Frisch, Hasslacher and Pomeau (FHP) introduced a lattice gas model based on hexagonal grids, this implies that there can be at most six particles per node. Rest particles also introduced into the model. There are three types of FHP models, i.e., FHP-I model, FHP-II model, and FHP-III model.

The FHP-II hexagonal lattice (there are six particles and rest particle on the node) is used as the basis of the model for the immiscible lattice-gas simulation of two-phase fluids separation and estimation of surface tension. All particles and holes are red and blue colored to distinguish the two fluids. For each direction at a given site assign a Boolean variable (f_i *(x,t),* N_i *(x,t)),* i = 1,2,…,6, for space x and time t, where N_i = 1 represents a particle and N_i = 0 a hole; f_i = 1 represents red particles and f_i = 2 represents blue particles. The bits with higher indices refer to the lattice directions c_i given by Equation (3). The collisions only occurs when the particles meet at the same lattice site at the same time, where the color flux is given by Equation (7), and the color gradient or color field is given by Equation (8), respectively. The conservation of the number of particles for each color and the conservation of total momentum during the collision process are (Chen, S *et al.* 1991),

$$\sum_i N_i f_i = \sum_i N_i' f_i' \tag{11}$$

$$\sum_i N_i (1 - f_i) = \sum_i N_i' (1 - f_i') \tag{12}$$

$$\sum_i N_i \mathbf{c}_i = \sum_i N_i' \mathbf{c}_i \tag{13}$$

where c_i is the unit velocity in the i direction, (i = 1, 2, …, 6).

The simulation of surface tension in two-phase fluids requires short-range attractive potentials between identical particles. To incorporate this attractive force, they let the particle collisions depend on the local color fields. A local flux introduced for the colored particles, G, and a local flux for holes, F, are given by equations (Chen, S *et al.* 1991; Rothman, D *et al.* 1997),

$$\mathrm{G} = \sum_i (2 f_i - 1) N_i \mathbf{c}_i \tag{14}$$

$$\mathrm{F} = \sum_i (2 f_i - 1)(1 - N_i) \mathbf{c}_i \tag{15}$$

Then, the surface tension estimated by using the Laplace's equation, (Chen, S *et al.* 1991),

$$\Delta p = p_r - p_b = \frac{\sigma}{L} \tag{16}$$

where p_r is the pressure of the red particles inside the drop, p_b is the pressure of the blue particles outside the drop, σ is the surface tension coefficient, and L is the radius of the drop. Pressure is calculated from the local density, ρ,

$$p = \frac{3}{7}\rho \tag{17}$$

Algorithms

The two different species in this simulation represented by two sets of particles, each being of a different color, i.e., red for gas and blue for oil, respectively. The particle collisions results depend on the phase distribution in the neighboring nodes. The collision rules change the configuration of particles so that, as much as possible, red particles are directed towards neighbors containing red particles, and blue particles are directed towards neighbors containing blue particles. The total mass, the total momentum, and the number of red or blue particles are conserved.

The algorithms for particle evolution, qualitative, and quantitative predictions are as follows:

1. Initialization
   In the initialization step, all parameters needed are defined in the program such as lattice size, the particle density, the ratio of red and blue particles, and time steps. Each type of particle arbitrarily distributed at the lattice sites. The directions of the particles are also randomly determined. The red and blue particle ratios are 0.2 to 1. Particle ratio is the ratio of the number of the red and blue particles (*dr/db*), if the ratio is 1 it means that the number of both types of the particles is the same or equal.
2. Input time steps
   Time steps are the sum of the iterations that are simulated.
3. Particles Propagation
   Particles in each lattice propagated into the nearest neighbor corresponding to their velocity directions. The number of particles is kept constant.
4. Particles Collision
   The collision in this model, for *n* greater than 1 then the configuration as the result of the first collision is the same with the configuration before collision. However, it will depend on the particles arrangement. Particles arrangement is change to classify the identical particles to the nearest particles neighbor, which contain the identical particles. Next, the output state is determined to maximize the quantity of Q = -F.G', where F is calculated from the given input hole state before a collision (Equation 15) and G' is calculated for the output particle state (Equation 14). This constraint ensures that the colored particles move in the direction opposite to the local color-hole flux:
   - If there are several configurations, G', which have the same maximum value of Q, then we choose the output having minimum $\left| G' \right|$. This step directs the colored particles as closely as possible in the opposite direction of the local color-hole flux and stabilizes the plane interface and the circular interface.
   - If there are still several possible configurations, then the output state with a rest particle was chosen. This slows the flow of the fluid and enhances phase separation.
5. Calculating density
   The calculation of density is a process to re-calculate color intensity and color gradient as the results of both propagation and collision steps.
6. Back to step 3 if *t* is less than time steps.

Results and Discussion

The immiscible lattice gas model had been develop for simulating two immiscible fluids using Borland Delphi-5 program. The FHP-II hexagonal lattice was use as the basis of the model for the immiscible lattice-gas simulation of two-phase fluids separation and estimating the surface tension on the 500x500 lattice sizes.

Fig. 3, illustrates how to recognize the interface between two fluids generated by immiscible lattice-gas model. The lattice sites were occupied by red components separate from the surface by six red-rich neighboring lattice sites. Similarly, the lattice sites occupied in blue components separate from the surface by six blue-rich neighboring sites. No-slip boundary conditions are applied to ensure that red particles entering the lattice, which has blue particles will bounce back in their opposite direction. The interface consists of a set of connected lattice sites and the motion of the interface at each link between adjacent lattice sites determined by the next momentum perpendicular to the link. After the interface had been moved, the number of particles of each color conserved by creating and annihilating particles with the same momentum near the interface. Effectively, the particles interact with each other over a distance of one or two lattice spacing across the interface. At each interfacial site, the interface moves in the direction given by the average momentum on the site and with probability equal to the magnitude of this average momentum. If a move results in a new lattice site, which cannot be connected, then the move is rejected. Qualitatively, surface tension is the result of the rules, which prohibits particles of one color from pointing towards lattice sites of the other color. From such a scheme, surface tension then can be deduced.

Simulation results of two-phase fluids separation are shown in **Fig. 4** through **Fig. 9**, respectively. The system displays for two-phase fluids separation has 500x500 lattice sites with periodic boundary conditions. The initial particles and hole color configuration is randomly distributed and the density, *d*, is 0.8 particle per direction. The ratio of red particles to blue particles, *dr/db*, is one, where *dr* and *db* are the red particles per state and blue particles per state, respectively. The particle ratio one it means that the number of both types of particles is the same. Each ensemble (10x10 lattice sites) described with a box on the display graphs.

Fig. 4 through **Fig. 9**, are describes the evolution of the particles to reach the steady state condition. **Fig. 4**, is the initial state, where red and blue particles distributed randomly. The red and blue drops in the figures stand for the red-riched lattice and blue-riched lattice, respectively. In the initial condition, the two component materials are completely random distributed. Two components start to separate and form complex interface geometry between the components as time marching. Because of Brownian motion of the color drops, the color drops gradually merge and form bigger drops. The final stable state is the minimum surface energy state, which has energy proportional to the length of the interface. **Fig. 5** and **Fig. 8**, are the condition where each same particles began to become merge, as physically this due to each same particles has a strength cohesion forces. **Fig. 9**, is the condition of the separation processes at 73000 time steps, the red and blue particles have separated forming a stable drop. It should be note that the immiscible lattice-gas model automatically generates the complex geometry of the interface. When the range of the interaction is large enough for a certain given values of density, the lattice gas separates into two phases. The growth of the bubble continues until an equilibrium state is reached where the two phases are entirely separated and the interface length is minimized. An interesting feature of the observed patterns is the asymmetry between high- and low-density regions. Another interesting effect is that momentum-conserving to yield separation. One of the reasons for this is that the surface tension effects yield faster domain growth in momentum-conserving systems. The mechanisms of growth a specific one involves bubbles undergoing Brownian motion, colliding, and being rapidly squeezed into a bigger, rounder and ellipsoidal shapes bubble by surface tension. Therefore, a few round bubbles are observed because the new bubbles collide again with each other. Beside that, isolated droplets also formed. The morphology of the pattern and the mechanisms of growth depend on the density.

Surface tension observed by plotting between pressures (p) as a function of distance (L) from the center of the drops as shown in **Fig. 10**. The pressure change at the interface of two immiscible fluids demonstrates the existence of surface tension. Surface tension is evident from the higher density inside the bubble. **Fig. 10**, also shows that pressure decrease at the distance, L, equal than 130. Then, surface tension can be estimated from the plotting between pressure difference (Δp) versus inverse distance ($1/L$) based on the Laplace's formula, i.e., given by the slope of the best fitting line that passes the origin data values. The result is shown in **Fig. 11**, where the value of surface tension (σ) is 0.00603. From all the results of the surface tension estimation demonstrates, the linear relation shows that the surface tension is a constant. The results summary is shows in **Table 1** and **Fig. 12**, respectively.

In enhanced oil recovery process, the interfacial and/or surface tension is one of the factors that affect the microscopic displacement efficiency. When a drop of one immiscible fluid is immersed in another fluid and comes to rest on a solid surface, the surface area of the drop will take a minimum value owing to the forces acting at the fluid-fluid and solid-fluid interfaces. The forces per unit length acting at the fluid-fluid and solid-fluid interfaces are referred to as interfacial or surface tensions. The interfacial or surface tension between two immiscible fluids represents the amount of work required to create a new unit of surface area at the interface. The interfacial or surface tension can also be thought of a measure of the immiscibility of two fluids.

Based on the simulation results, it is shows that the immiscible lattice-gas model applicable to simulate numerically of two-phase immiscible fluids as an alternative method of laboratory experiments. Phase separation of two immiscible fluids can be simulated and the surface tension had been estimated.

Conclusions

1. The lattice-gas model for two-phase immiscible fluids has been developed.
2. The separation of two fluids that have a different density can be simulated.
3. The same particles of two immiscible fluids began to become merge due to cohesion forces.
4. The pressure change at the interface of two immiscible fluids demonstrates the existence of surface tension.
5. The surface tension between two immiscible fluids can be estimated.
6. The simulation is also allows us to model fluid-fluid and fluid-solid interactions.

Nomenclature

b' = post-collision states of blue particle
c_i = the unit velocity in the i direction (i = 1, 2, …, 6)
f = color gradient or color field
F = local flux for holes
G = colored particles
L = radius of the drop
p_r = pressure of red particles inside the drop
p_b = pressure of blue particles outside the drop
p = pressure
Δp = pressure differences
q = color flux
r' = post-collision states of red particle
s = color state of two-dimensional ILG
t = time
x = lattice space
σ = surface tension coefficient
ρ = local density

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TABLE 1- ESTIMATION OF SURFACE TENSION RESULTS SUMMARIZE ON THE 500x500 LATTICE SIZES FOR EACH PARTICLE RATIO (dr/*db*)

Particle Ratio (*dr/db*)	Surface Tension (*σ*)
0.2	0.00585
0.4	0.00588
0.6	0.00598
0.8	0.00600
1.0	0.00603

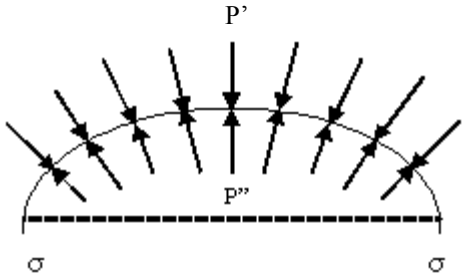

Fig. 1- Capillary equilibrium of a spherical cap, (After Dullien, 1979).

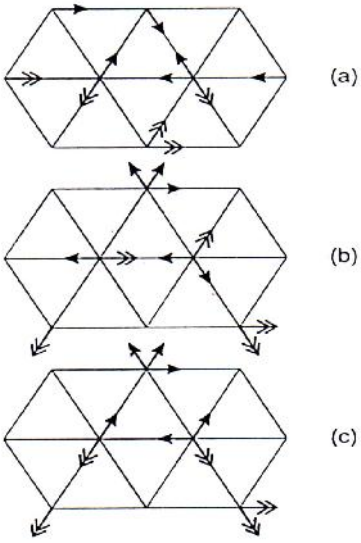

Fig. 2- Evolution of the immiscible lattice-gas model, where (a) is the initial condition, (b) is the propagation step, and (c) is collision step. In the collision step, the particles are re-arranged so that, the flux of color is in the direction of the local gradient of color, (After Rothman, D *et al.* 1988, 1997).

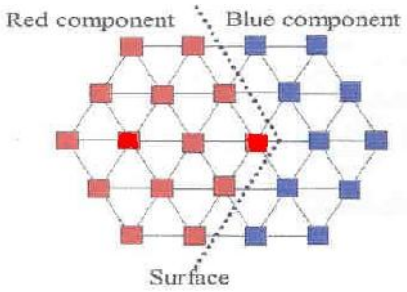

Fig. 3- Schematic that illustrates the lattice states near the surface of red and blue components for a given time steps.

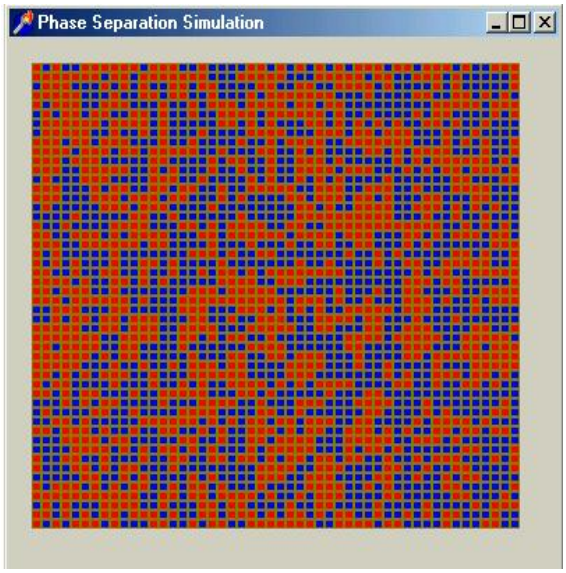

Fig. 4- Phase separation evolution results on the 500x500 lattice sizes, *dr/db* = 1, at t = 0 time steps.

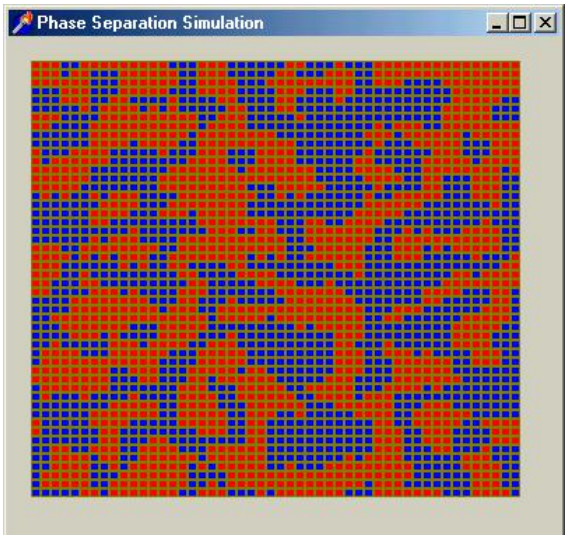

Fig. 5- Phase separation evolution results on the 500x500 lattice sizes, *dr/db* = 1 at t = 10000 time steps.

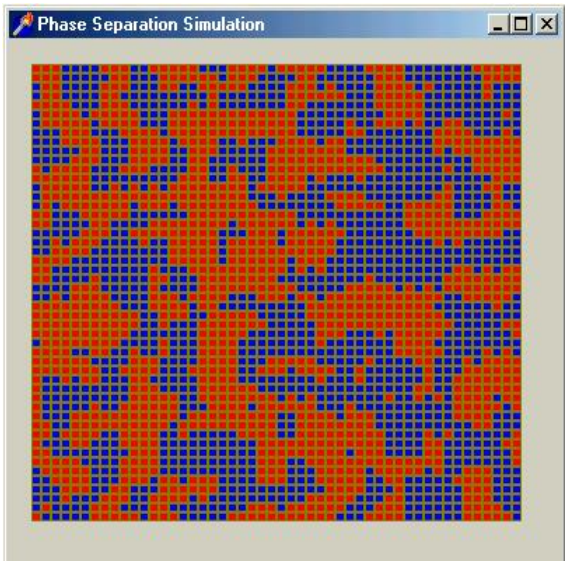

Fig. 6- Phase separation evolution results on the 500x500 lattice sizes, *dr/db* = 1, at t = 23000 time steps.

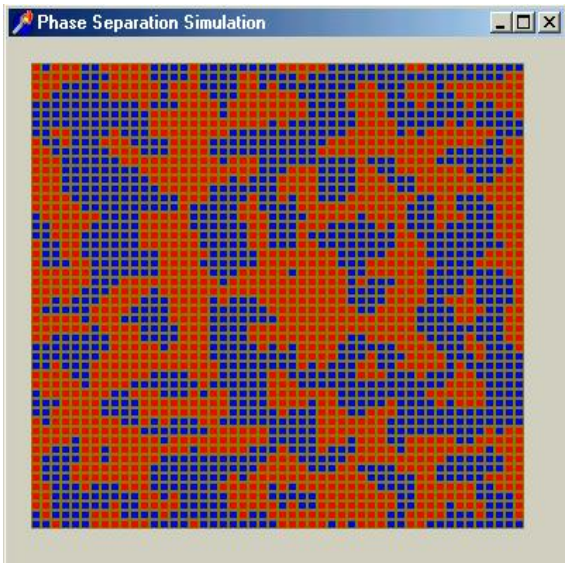

Fig. 8- Phase separation evolution results on the 500x500 lattice sizes, *dr/db* = 1, at t = 46000 time steps.

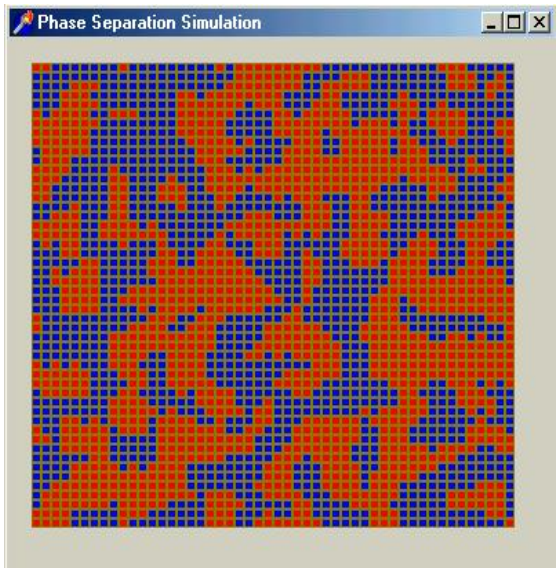

Fig. 7- Phase separation evolution results on the 500x500 lattice sizes, *dr/db* = 1, at t = 35000 time steps.

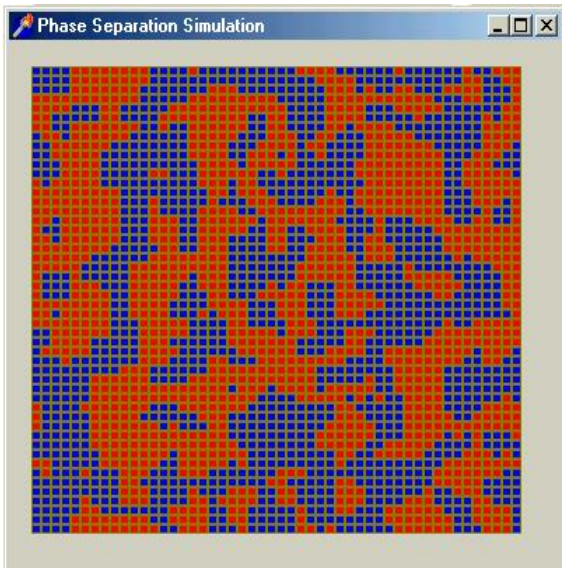

Fig. 9- Phase separation evolution results on the 500x500 lattice sizes, *dr/db* = 1, at t = 73000 time steps.

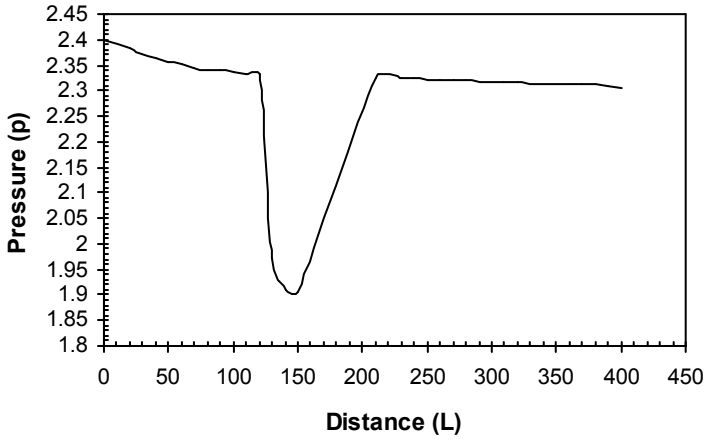

Fig. 10- The typical pressure distributions as a function of distance (*L*) from the center of the bubble.

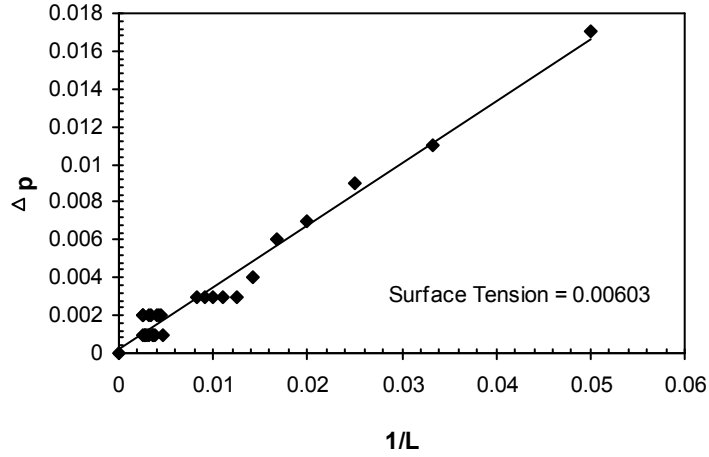

Fig. 11- The simulation results of pressure difference (Δp versus 1/*L*) across the bubble for different radii.

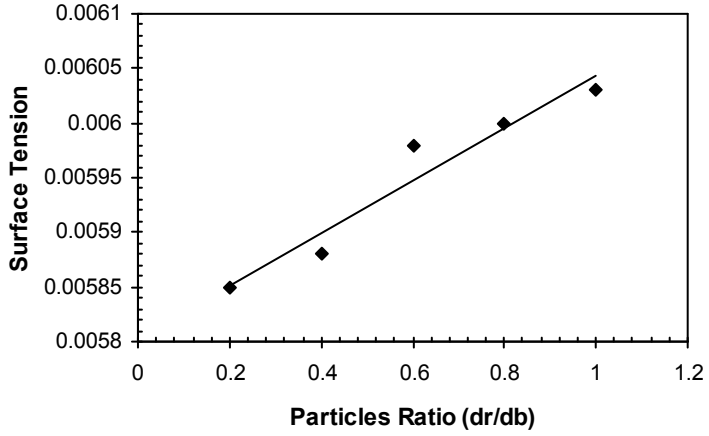

Fig. 12- The summary of simulation results of surface tension estimation for each particles ratio (*dr/db*).