Simulation of phase separation by the two-phase shallow water equations

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1. Introduction

The purpose of this research is to develop a simulation method for pattern formation by phase separation in the liquid film. The phenomenon of phase separation is formulated by the two-phase flow equations. As the scale of the vertical direction is different from the horizontal direction in the liquid film, the shallow water approximation is effective. Appling the shallow water approximation to the two-phase flow equations, a new system of equations, named the two-phase shallow water equations, was derived. As for phase separation, the order parameter is calculated by the equations of fluid dynamics. Driving force of the phase separation is the gradient of chemical potential formulated by the order parameter. In this point, the formulation is different from phenomenological equations.

Simulations are performed by the new invariant finite difference scheme. As for pattern formation, invariance of the coordinate transformation, such as the Galilean transformation or the similarity transformation plays an important role. At first, one dimensional invariant scheme was constructed. Then the scheme was extended to the two dimensional case by the locally one dimensional method(LOD). The Numerical experiments were performed to the problem of evaporation induced phase separation.

2. Formulation

A New equations are derived from the equations of the two-phase flow by the shallow water approximation(3). When the two-phase flow consists of C-phase and D-phase, the independent variables of the two-phase shallow water equations in one dimension are surface height, x-direction velocity of C-phase and D-phase, volume fraction of one phase. The sum of volume fraction of C-phase and D-phase equals unity. The velocities of the equations are horizontal.

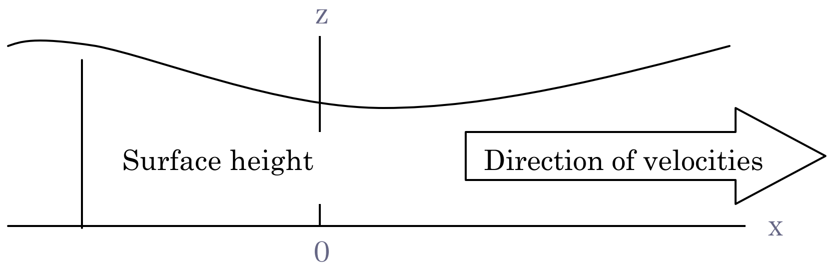
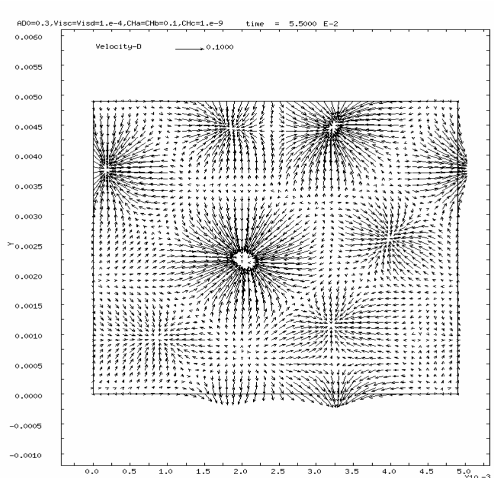
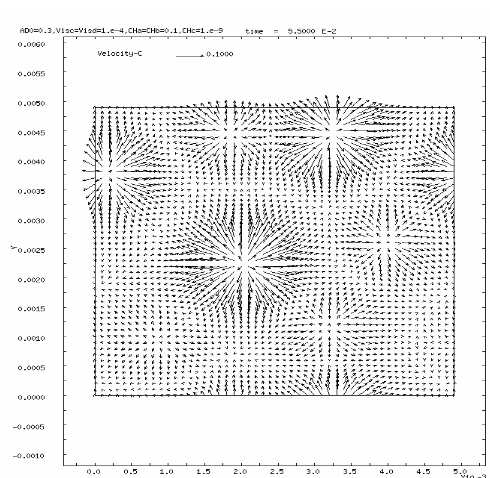


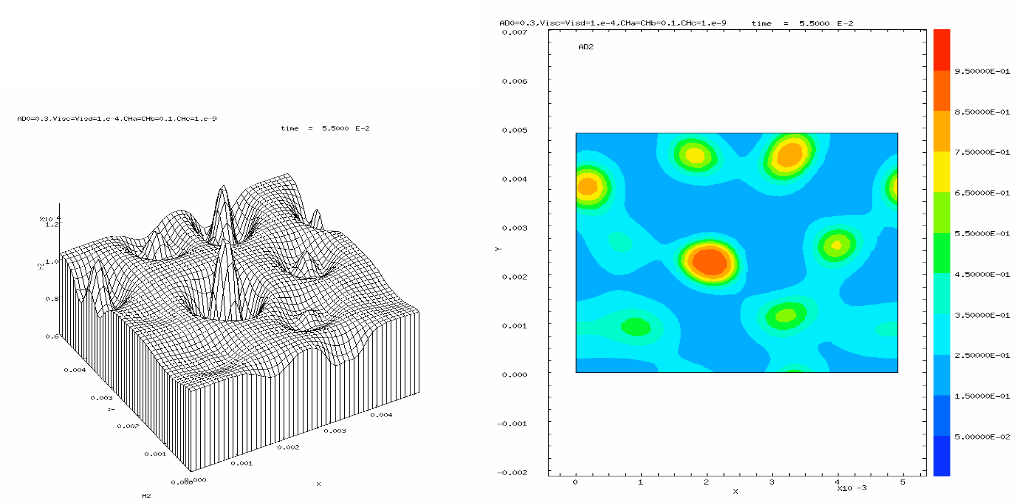
Fig.1 The sallow water approximation

To simulate the shape of the surface precisely, invariance of the coordinate transformation plays an important role. A finite difference scheme whose first differential approximation is invariant to the transformations is called invariant finite difference scheme(1). A new invariant finite difference scheme of the two-phase shallow water equations proposed in the one dimension(3). Then the scheme of was extended to the two dimensional case(4). The form of the one dimensional scheme is complex. And the system of two-phase shallow water equations is non-symmetric hyperbolic. The two dimensional scheme was constructed by LOD for the simplicity and to guarantee the stability of the finite difference scheme. But the proposed scheme loses the invariance of rotational transformation in the two dimension. To recover the invariance of rotational transformation, two schemes are averaged in which the order of one-dimensional calculations is different. In spite of the system of equations is quasilinear, this works well like linear case(2). An example of the simulation is shown below.





Velocity of C-phase Velocity of D-phase

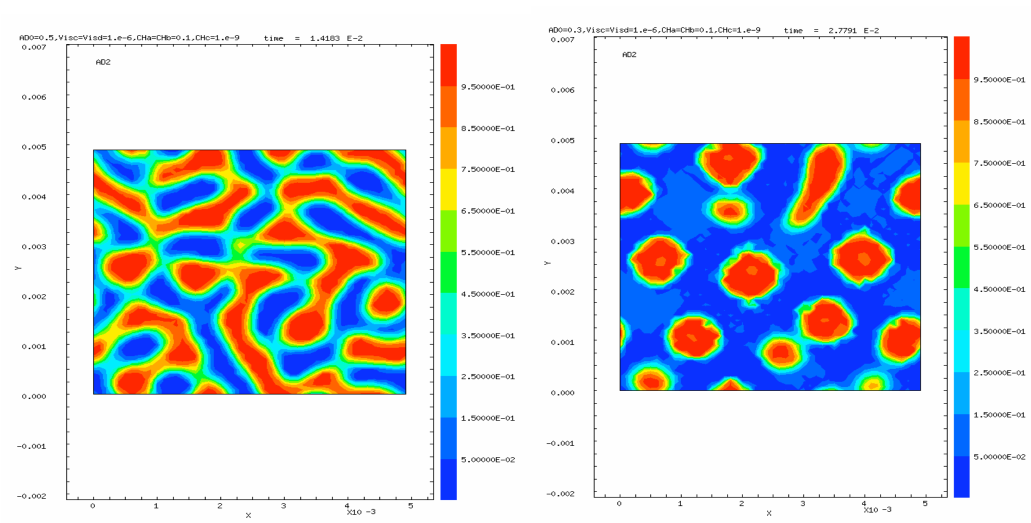


Surface height（×100）　　　　　　　　Volume fraction of C-phase

Fig.2 Variables of simulation by the two-phase shallow equations

3. Simulation of phase separation

Phase separation in the thin film of liquid binary mixtures is studied numerically. The model is the two-phase shallow water equations with dri ving force of phase separation based on the Ginzburg-Landau free energy. Numerical experiments are performed to investigate the effects of the volume fraction on phase separation. As is well known, patterns are different according to the ratio of the volume fraction. Results are below.

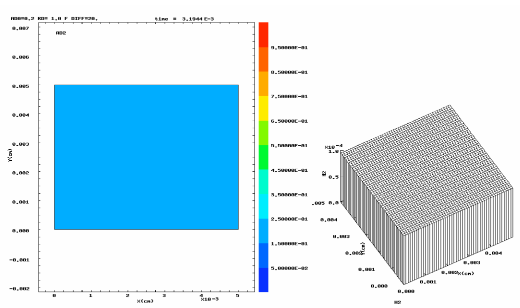


C-phase:0.5 D-phase：0.5　　　　　　　　C-phase:03 D-phase:0.7

Fig.3 Patterns of phase separation

A simple analysis of the two-phase shallow equations can show that phase separation does not appear, if densities of both phases are equal and the volume fraction of one phase is smaller than 1/2(1-1/sqrt(3)) or bigger than 1/2(1+1/sqrt(3)).

When C-phase is volatile, the volume fraction of the liquid film changes continuously. Even if C-phase is rich and the state of the liquid film is uniform in the early stage, phase separation appears in the medium stage. So the surface may not flat in the late stage as below.



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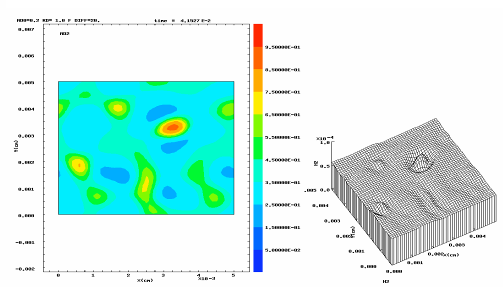

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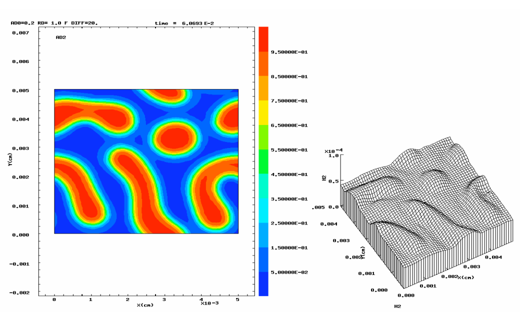

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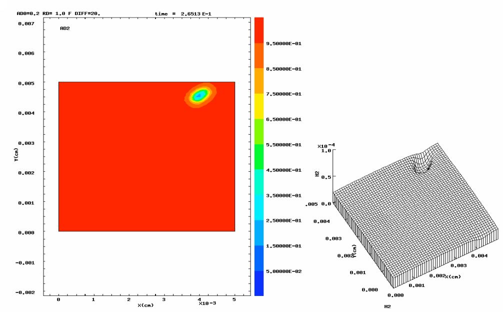

time=0.26

Fig.4 Simulation of evaporation induced phase separation

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