Cahn-Hilliard Simulation

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discretization procedure is subtracted numerically and the concentration at the boundary is set to the average of the two initial conditions. The non-linear Cahn-Hilliard (CH) equation with chemical potential was then solved numerically using a finite difference method. The resulting numerical solutions were then compared against the analytical solutions to validate the discretization procedure. The resulting numerical solutions were then compared against the analytical solutions to validate the discretization procedure. The resulting numerical solutions were then compared against the analytical solutions to validate the discretization procedure.

For our numerical simulations, the two-dimensional Cahn-Hilliard (CH) equation was solved for various values of \( \phi \), ranging from 0.5 to 0.95. Each solution was obtained using the forward Euler scheme with a time step of \( \Delta t = 0.001 \) and a space step of \( \Delta x = 0.001 \) for a total of 1000 time steps. The concentration at the boundary was set to the average of the two initial conditions. The non-linear CH equation with chemical potential was then solved numerically using a finite difference method. The resulting numerical solutions were then compared against the analytical solutions to validate the discretization procedure. The resulting numerical solutions were then compared against the analytical solutions to validate the discretization procedure.

In each case, the initial conditions were chosen by assigning each node a value of \( \phi \) chosen using a Gaussian distributed random number generator with mean value \( \langle \phi \rangle \) and a standard deviation of \( \sigma \). For each \( \phi \), 50 random initial conditions were created and the CH equation was solved for each condition.

Independently the early data of \( \phi \) was analyzed. For each composition the data were collected at a series of times as \( \phi_{0} = 1.0000 \), \( \phi_{1} = 1.0000 \) and \( \phi_{2} = 1.0000 \). To investigate the effect on the time evolution due to \( \phi_{0} \) and the standard deviation of the random distribution of the initial conditions, simulations were carried out at \( \phi_{0} = 0.01 \), \( \phi = 0.02 \), \( \phi = 0.05 \) and \( \phi = 0.1 \). 50 runs were carried out for each \( \phi_{0} \), \( \phi_{1} \), \( \phi_{2} \), and \( \phi_{3} \) and 10 runs were made for each \( \phi_{4} \) and \( \phi_{5} \). The standard deviation of the random distribution is \( \sigma = 0.01 \) for all the simulations.

The rate of change of slope of the graph in Fig. 5 is maximum as \( \phi \) goes from 0.0 to 0.1. This is the region where the CH model deviates most from the initial solution. This further indicates that there is a critical region of \( \phi \) which acts as a boundary for the two regimes.

Discussion

One end of an oil molecule is hydrophilic while the other is hydrophobic. When two fluids with different chemical properties, such as oil and water, are mixed then the enthalpy of the homogeneous state is greater than the separated state. Under these conditions, interfacial variations in the local composition of the mixture lower its free energy and lead to phase separation. This is called spinodal decomposition which takes place at a very early stage of the separation process. In the initial decomposition, the two components separate into regions containing dominantly one type of fluid. In the late stage, surface tension is the driving force for domain coarsening. The Lifshitz-Slyozov model does not account for cluster correlations. For greater \( \phi \), the cluster interactions are reduced, so the LS prediction is more likely to be valid. For smaller \( \phi \), cluster interaction is stronger is the early stages, resulting in correlated, non-circular domains (see Fig. 1). Thus, for different \( \phi \), the scaling regime is different. The scaling regime is the time interval where the blobs slowly grow in size rather than change shape. This is the region where the LS relation is expected to be valid. The measure of non-circularity, \( q \), is used to determine the scaling regime during the phase separation. This is affected by the shape of the blob and not the size. Thus, the scaling regime is set to be reached if \( q \) stops changing with time. Eqn. 1 assumes that the only force acting on the two components of the mixture is the inter-molecular force due to the different solubility. Thus the simulation of the CH equation requires that the size of the domain be infinitely large as compared to the blobs. For the grid size of 100x100 the periodic boundary condition influences the time evolution of the minority regions. For 540x540 grid size the boundaries had less effect. Thus the time evolution of the blobs show the LS behavior more closely. Also for the smaller grid size, a smaller number of blobs are produced which quickly forms into a single blob making it more difficult to investigate the phase change characteristics.

When \( \phi \) is smaller, the blobs are concentrated into points at the initial time step. The average blob separation is large. Thus it takes some time for them to get organized into larger blobs. Whereas for larger \( \phi \) the blobs at the initial stage are more likely to grow faster and connect by the neighboring blobs. Thus, they quickly form larger blobs and grow faster in time as compared to the mixtures with smaller \( \phi \).

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References: