Monte Carlo Simulation of the Percolation Phenomena in Water-in-Oil Nano-Emulsion

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Abstract:

In this study, Monte Carlo simulation was used to model the electrical percolation behavior in a two phase water-in-oil system. The relationship between conductivity and water content was verified using the 3-dimensional model. The observed phenomena was modeled using –unit cells. The minimum volume fraction of water necessary for complete connection increased with the decrease in the size of the unit cell.

1. INTRODUCTION

First, what is Monte Carlo? "Monte Carlo method" is based on the use of random numbers and probability statistics to investigate problems. In the water-in-oil nano-emulsion system, water droplet dispersed in the continuous oil medium, and this nanoscale droplet is used as nano reactor in producing nanoparticles, such as metal, oxides particles. In this simulation, the nano-emulsion system was assumed as a mixture of an insulator (oil medium) and a conductor (water droplet), the droplet was random dispersed in the oil medium.

2. OBJECTIVE

The overall objective was to investigate the feasibility of using Monte Carlo simulation method to investigate the percolation behavior in water-in-oil nano-emulsion system.

3. SIMULATION

3.1 2-Dimensional lattice simulation: In 2-dimension case, the mixture was simulated on an L×L two dimensional square of lattice; L=25 was chosen for most of calculations. Each water droplet occupies a single lattice site. For a given system containing Nw water, and the oil molecules act as a uniform background occupy a total of No=N-Nw sites, where $N=L^2$ is the total number of sites in the lattice. Each water droplet moves at random, so a random distribution of the water droplets can be illustrated as 2-D random checkerboards as Figure 1. The main variable is the unit cell size and its effect on the percolation threshold.

3.2 3-Dimensional cubic lattice simulation: A 3-dimensional numerical calculations were also performed. In the calculation, the water droplets were assumed be randomly distributed in the cubical lattices, see Figure 2. The droplets (conducting phase) then appear in the shape of unit cubes, and randomly fill the blocks, and then insulating medium will fill the empty block after that. Different arrangements were, therefore, used in attempt to emulate realistic systems. Two parameters were investigated, one is the unit cell size, another one is the conductivity ratio of the water to oil phase.

4. RESULTS AND DISCUSSION

4.1 Effect of the number of unit cell size: The percolation behavior was more obvious as the number of unit cells was increased. The volume fraction of water at which connectivity was first observed was shown in percolation increased upon decreasing the size of unit cell, as shown in Figure 3.

4.2 Effect of conductivity ratio of two phases: The addition of surfactant may change the conductivity of both oil medium and water medium. By running the program with different conductivity ratio, it was possible to develop the relation between the water content and the system's conductivity. By comparing the calculation results and the experimental results, we can obtain the estimated ratio between the two phases. The model and experiment showed that increasing the surfactant concentration increased the conductivity ratio between the two phases.

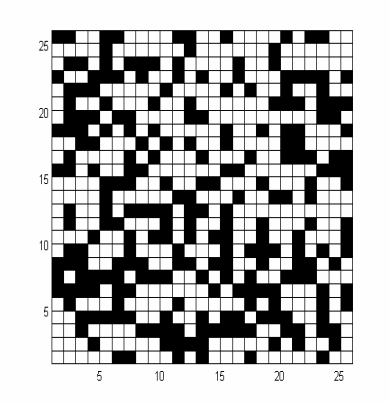

Fig.1 Schematic of water droplet distribution on a 2-D 25 ×25 square lattice (Occupy probability=39%, percolated)

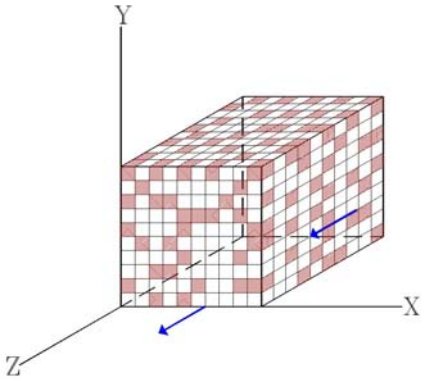

Fig.2 Schematic of water droplet distribution in 3-D 10 ×10 ×10 cubic

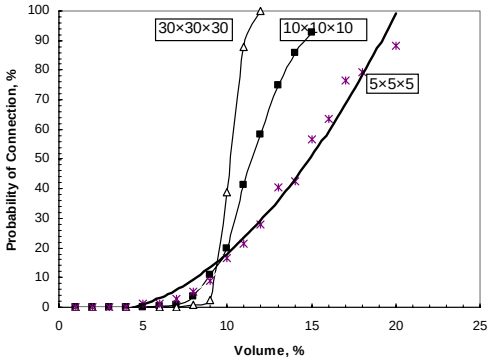

Fig.3 Probability of connection for different numbers of unit cells (3D)

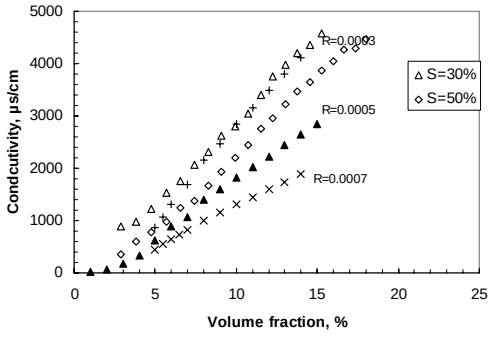

Fig.4 Simulation results of different conductivity ratio of the two phase compared to the experimental results

5. CONCLUSION

The Monte carlo simulation method was effective in investigate the percolation behavior of the water-in-oil nano-emulsion system. The effects of unit cell size and conductivity ratio between the two phases on the percolation phenomena were investigated.

6. ACKNOWLEDGEMENT

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7. REFERENCES

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