外国語要旨

Prediction of emulsified droplets and nanoparticles production in microchannel
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1. Introduction

Micromaching techniques have been adopted in the design of miniaturized devices, e.g. microreactors, for chemical synthetic applications. A microreactor is a device in which chemical reactions can be performed carried out on a microscale. The potential advantages of using microreactor, rather than a conventional batch reactor, are as follows: the fluids to be mixed have a laminar flow, and mixing progresses rapidly because of the short diffusion length of the materials in the microreactor.

Because of these advantages, recently, microreactors have been used to product emulsified droplets and nanoparticles. The emulsified droplets and nanoparticles are widely used as materials for chemical industrial products in recent years. Here, the emulsified droplets and nanoparticles are required uniform and small sizes. Therefore, we applied microreactors to obtain high quality products.

2. Methods

We have developed a microreactor system for the production of emulsified droplets and AgCl nanoparticles. The research method is as follows.

1) To simulate the emulsification process in a micro-channel, a computational fluid dynamics (CFD) technique, called the volume of fluid (VOF) method, was used.

Based on the simulation results, a uniform emulsified droplet production range was predicted using dimensionless numbers.

2) We evaluated the mixing performance of a microfluidic device quantitatively by CFD for the purpose of estimating uniform nanoparticle production conditions.

Based on the simulation results, we quantitatively predicted AgCl nanoparticles production process in the microchannel.

3. Resutls and discussion

To estimate emulsified droplets and nanoparticles production conditions, we applied CFD. As a results, it came to following conclusions.

1) It was confirmed that the length of droplet position determined by the VOF method agrees well with the experimentally measured within an error of 15%.

In accordance with that agreement between calculation and experiment, a map of the generation of uniform emulsified droplets was constructed by using the VOF method.

The map is defined by two dimensionless parameters: Reynolds number (*Re*) and Capillary number (*Ca*). It is clear from the map that the generation of droplets peaks at *Re* of 3.0 to 4.0 and *Ca* of 10.0×10^{-3}.The map makes it possible to generate emulsified droplets experimentally within a coefficient of variation (Cv) of 5 %.

2) We compared the mixing performance between experimental and simulation results using five microreactors. We clarified that the simulation results for evaluating mixing performance were in good agreement with the experimental results. Therefore, we confirmed that CFD can be applied to prediction of mixing performance of microreactors.

Next, we applied CFD results for evaluating mixing performance to estimation of AgCl nanoparticle production process. We have found that the particle size of nanoparticles correlates with the residence time of microreactor system. The particle size increased from 66 nm to 243 nm with the increase of the residence time from 15 s to 120 s. Furthermore, we clarified that the particle size distribution of AgCl nanoparticles was related to the mixing performance of the microreactor. We confirmed that the mixing time of two solutions was shorter than 10^{-6} s, and we achieved Cv (Coefficient of Variation) of less than 30 %. Therefore, we confirmed that the condition of nanoparticles production was able to be estimated by applying CFD to the mixing performance evaluation of microfluidic devices.

From the above results, we confirmed that the condition of emulsified droplets and nanoparticles production process can be estimated by applying the fluid dynamics simulation to predicting the flow state in the microchannel.