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Computational Fluid Dynamics of Crystallization Process and Modeling of Nucleation in a Stirred Vessel

Ryuta MISUMI, Kazuhiko NISHI, Meguru KAMINOYAMA

National University Corporation Yokohama National University

Summary

In a crystallization process, estimation of crystal particle attrition occurred by impact on solid surfaces in a stirred vessel is important to stable operation of the crystallizer, and to control of the particle size distributions.

In this study, we performed the particle Lagrangian simulations coupled with CFD (Computational Fluid Dynamics) to calculate the statistical data of the particles impact position, probability and kinetic energy when they impact on impellers, wall and baffles in the vessel. Then, the stochastic analysis method of particle attrition phenomena based on the statistical data was established to calculate the long time attrition phenomena as seen in the industrial crystallization. Assuming the case of sodium chloride in xylene, attrition model parameters were decided based on verification experimental data. With this stochastic analysis, we can calculate the attrition phenomena for 10 hours with much shorter calculation time than that with the Lagrangian simulation.

Primary nucleation in crystallizer is very sensitive phenomena easily disturbed by impeller stirring, temperature fluctuation, intrusive sensors and impurity. So, we tried to establish a non-intrusive on-line measurement method of initial dynamic behavior of primary nucleation and growth with laser scattering method. Property of laser scattered light by particles suspended in a vessel was investigated under various size and mass conditions of polystyrene particles. The result shows that (a) the scattered light power has a positive correlation with amount of particles under dilute concentration, and reaches to maximum value, and (b) the maximum value of scattered light power has a negative correlation with particle size in case of hundreds nanometers or more in the particle diameter.

With these results, in future, we aim to the simulation of crystallization processes for long time, and to apply the non-intrusive measurement method to quantification of initial dynamics of the primary nucleation in the crystallizer.