Development of a method of numerically analyzing the crystallization flow field for the production of high quality crystals in a stirred vessel

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Summary

Crystallization is frequently used as a manufacturing process in many industries, such as pharmaceuticals, general chemicals and synthetics, and food, and the demands on the quality of the crystals produced have become severe, such as polymorphism and crystal shape, mono-dispersion of crystal diameter, average diameter and the level of refining. The establishment of a new method of accurately estimating and controlling the crystals produced in a stirred vessel is, therefore, strongly desired.

The purpose of this study is to develop a method of numerically analyzing the crystallization flow field, which is fundamental for the numerical analysis of the crystallization reaction process. Firstly, we developed a method of numerically analyzing the motion, in a Lagrangian way, of crystals floating in a stirred vessel. Further, we developed a method of analyzing the process of the crystal dissolution based on the instantaneous values of the slip velocity between each crystal particle and the liquid around the particle. Finally, we verified the reliability of these methods by observing the crystal dissolution process.

A numerical analysis was conducted for the dissolution of KCl crystal particles with a diameter distribution ranging from 150 to 200 μ m in a stirred vessel fitted with a 6-blade paddle impeller. The governing equation is composed of the Navier-Stokes equation, the Lagrangian equation of motion of particles and the transportation equation for the solute, KCl. We incorporated a correlation equation for the mass transfer coefficients ($Sh = 2.0+0.6(Re_p)^{1/3}(Sc)^{1/2}$) into the analysis scheme with an approximation of the spherical shape of the crystal particles. We verified the numerical analysis by measuring the dynamic changes in the average bulk concentration of KCl injected into a stirred vessel with an electric conductivity meter, under the same conditions as used in the numerical analysis.

We could specifically represent the motion of each crystal particle in the stirred vessel by the analysis, as well as analyze the dynamic changes in the solute concentration distribution and in the diameter of each particle in the vessel. The results obtained from the numerical analysis of the dynamic changes in the average solute concentration in the process, from crystal injection to complete dissolution, were essentially coincident with the data obtained from the verification experiments. We would like to extend the method of analysis of crystallization flow and dissolution established in this study to the numerical analysis of the crystallization reaction process.

In this study, we established a method of numerically analyzing the crystallization flow field and crystal particle dissolution process in a stirred vessel as a necessary, preliminary step towards developing a method of numerically analyzing the crystallization reaction process in a stirred flow field.