STOCHASTIC ANALYSIS OF ATTRITION PROCESS AND CRYSTAL SIZE DISTRIBUTION IN CONTINUOUS CRYSTALLIZERS

By

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ABSTRACT

The present study involves application of Monte Carlo technique for analysing complex problems of attrition process and crystal size distribution (CSD) analysis. For the former problem, it focuses on the effects of attrition on the theoretical CSD, modelling of experimental CSD results in a mechanically agitated crystallizer under attrition conditions and finally the effects of volume shape factor dispersion on the CSD resulting from attrition. While for the latter, it includes the simulation of transient CSD under size-dependent growth rate and stochastic dispersion effects for an imperfectly mixed crystallizer. The basic idea behind employing stochastic methods to handle aforesaid problems is that it obviates the need to solve the system equations, which often comprise coupled differential equations. Moreover, these equations often contain variables that render the analysis extremely complex.

In transient CSD analysis, the simulation scheme is attractive due to its simple algorithm, i.e. free from iterative calculations and related convergence problems. The simulated transient CSD can account for size-dependent growth. It could also incorporate improper mixing conditions under all possible dispersion effects. The agreement among the predicted results and available experimental data confirm the validity of the proposed scheme.

In the attrition process, MC offers an alternative to the conventional deterministic approach in solving the Random Breakage model, described by a second order ODE. In addition, a comparison between experimental CSD results under attrition conditions with the simulated CSD indicates good agreement. The MC method was also successfully used together with a physical model for obtaining the fragment size distribution. The distribution provides an account of the volume shape factor dispersion, which previous authors often, assumed to be a constant.

LIST OF PUBLICATIONS

1. K. C. Lim, M. A. Hashim and B. Sen Gupta, "Monte Carlo Simulation of Transient Crystal Size Distribution in a Continuous Crystallizer Using the ASL Model", Crystal Research and Technology (Akademie Verlag, Germany), **33** (1998) 2 pp. 249-255.[+]

2. K. C. Lim, M. A. Hashim and B. Sen Gupta, "The Effect of Volume Shape Factor on the Crystal Size Distribution of Fragments due to Attrition", Crystal Research and Technology (Akademie Verlag, Germany), **34** (1999) 3 pp. 491-502.[+]

3. K. C. Lim, M. A. Hashim and B. Sen Gupta, "Transient Crystal Size Distribution in DTB and FC Crystallizers", Crystal Research and Technology (Akademie Verlag, Germany), **34** (1999) (Accepted for Publication). [+]

4. K. C. Lim, M. A. Hashim and B. Sen Gupta, "Monte Carlo Simulation of Transient Crystal Size Distribution in an Imperfectly Mixed Continuous Crystallizer under Stochastic Dispersion Effects", International Mixing and Crystallization Conference, Pulau Tioman, Malaysia (1998).

[+] The papers are included in the back cover.

5. K. C. Lim, M. A. Hashim and B. Sen Gupta, "Monte Carlo Simulation of Crystal Size Distribution with Attrition Effects in a Mixed Suspension Crystallizer", International Mixing and Crystallization Conference, Pulau Tioman, Malaysia (1998).

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INTRODUCTION

Deterministic analysis of attrition process and transient crystal size distribution (CSD) is a difficult task owing to the complexity of the basic population balance equation (PBE). Often, the solution is very difficult except for simple cases. Alternatively, one could employ the stochastic analysis in solving the PBE that could easily account for growth rate dispersion, size-dependent growth, shape factor dispersion, birth size dispersion and change in nucleation rate simultaneously. These considerations introduce non-linearity in the PBE in the conventional deterministic approach and a lack of mathematical tool has been a major impediment in solving these equations.

Two different stochastic methods are commonly employed to predict the behavior of the CSD, namely the Markov process and the Monte Carlo (MC) technique. The basic advantages of the Markov process over the MC simulation are as under:

(i) CSD's are available on a continuous time scale.

(ii) It is more efficient with respect to computation time for the simple cases that it can handle.

Unlike the Markov process, the simulation results obtained from the MC simulation are discrete on a time scale. However, due to the following remarkable

features, MC technique has been recognized as a more versatile tool than the Markov process:

(i) One can account for the influence of shape factor dispersion on CSD.

(ii) The CSD can be expressed as both number and mass fractions for steady and non-steady state conditions.

(iii) One can use any statistical density function to represent the dispersion effects.

(iv) The simultaneous dispersion in growth, shape factor, nucleation rate and birth size can be accounted for in the calculation of steady state and transient CSD's.

(v) It is a direct simulation technique and is free from any iterative calculations.

The present contribution involves application of MC technique to handle complex problems of transient CSD analysis (Chapter 2, 3, and 4 of Part 2). In addition, the MC is also employed to simulate the CSD of crystals as the result of attrition processes (Chapter 5, 6, and 7 of Part 3). For the former problem, it includes the simulation of transient CSD under size-dependent growth rate and stochastic dispersion effects for an imperfectly mixed crystallizer. While for the latter, it focuses on the effects of attrition on the theoretical CSD, modelling of experimental CSD results in a mechanically agitated crystallizer and finally the effects of volume shape factor dispersion on the CSD of fragments generated from a mechanically stirred crystallizer.

In Chapter 2, the transient CSD is simulated using the MC method under size-dependent growth rate conditions. The classical approach in simulating the CSD in a continuous mixed suspension mixed product removal (MSMPR) crystallizer is based on several hypotheses. A very important assumption is the constant growth rate of the crystals known as McCabe's delta L law. However, there is ample evidence that growth rate is a function of size in some systems. Under the present work, a MC simulation scheme is proposed for transient CSD in a continuous crystallizer to account for size-dependent growth rate. Crystal growth rates are described by ABEGG, STEVENS and LARSON (ASL) model. The proposed model is used to predict the transient CSD from potassium carbonate crystallizer. The agreement between theory and available data confirms the validity of the model.

In Chapter 3, the transient analyses of CSD for an imperfectly mixed draft tube baffled (DTB) and forced circulation (FC) crystallizers are predicted using the MC technique. To account for the non-ideal mixing conditions, the DTB and FC crystallizers are described by the compartmental and mixed models respectively. The simulation results have been compared and agreed with the available experimental data of BENNETT and VAN BUREN (1969) for continuous urea crystallizer. This work has been further extended in Chapter 4 to forecast the transient CSD in a crystallizer for simultaneous dispersion effects in growth rate, shape factor and birth size. It also takes into account the possible variation in nucleation rate in a crystallizer. The earlier work of SEN GUPTA and DUTTA (1991) has been used to validate the results.

In Chapter 5, the effect of attrition on the CSD in a continuous mixed suspension crystallizer was predicted by a Random Breakage model as proposed by RANDOLPH (1969). The CSD was computed by MC technique and compared with the deterministic solution of the PBE proposed by RANDOLPH (1969). The agreement between the two approaches confirms the validity of the MC technique.

Chapter 6 reports the experimental work carried out to determine the CSD resulting from breakage and abrasion occurring in agitated crystal suspensions. The effect of two operating variables, i.e. duration of run (≤1 hour) and low stirring rates (≤ 400 rpm) are shown with reference to sodium chloride crystals. The experimental results were used to validate the model proposed by MAZZAROTTA (1992) and BISCANS *et al.* (1996).

The effect of volume shape factor on CSD is usually ignored to simplify the analysis of PBE. In Chapter 7, the CSD of fragments generated from a mechanically stirred crystallizer as the result of attrition mechanism has been reported. The physical model of GAHN and MERSMANN (1997) which relates the attrition resistance of crystalline substances to its mechanical properties has been employed with suitable modification. The simulation of fragment size distribution was performed by MC technique.