

enabling technology for high performance crystallization process development and design. This chapter aims to give a brief but comprehensive overview of PBM based description of crystallization processes.

The chapter starts with an introduction describing the modeling of fundamental crystallization mechanisms, followed by a brief description of the modeling of mixed suspension mixed product removal (MSMPR) crystallizers and plug flow crystallizers (PFC). A high-level description of the most commonly used numerical solution techniques is presented, and at the end of the chapter demonstrative examples are given for advanced population balance-based crystallization models, which include topics such as modeling of solvent mediated polymorphic transformation, preferential crystallization and growth rate dispersion.

2.2 Modeling of Fundamental Crystallization Mechanisms

Crystallization is a dispersed phase process where the crystals or the solid phase are dispersed in solution as continuous phase. The various subprocesses that can be present in the crystal phase are growth, nucleation, dissolution, aggregation and breakages as shown in Figure 2.1. While nucleation, growth and dissolution involve mass transfer between the continuous and dispersed phases, aggregation and breakage are purely due to the crystal-crystal interactions. The changes in the crystal phase resulting from the aforementioned processes are tracked by the population balance equations (PBEs). On the other hand, the changes in the continuous phases (*e.g.*, concentration and temperature) are tracked by mass and energy balance equations. These changes that take place due to mass transfer and

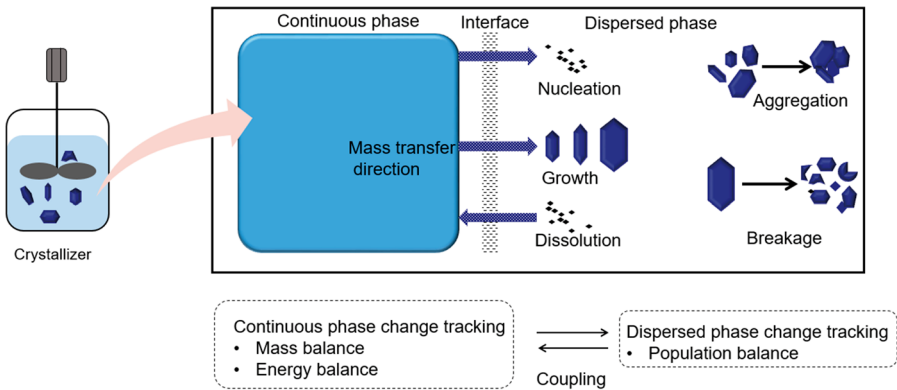


Figure 2.1 Schematic diagram showing the various subprocesses present in crystallization processes. Population balance modeling tracks the changes in the dispersed phase (*i.e.*, crystals) while mass and energy balance equations track the changes in the continuous phase (*i.e.*, solution). These two sets of equations need to be coupled for describing the crystallization process.⁵