Dynamic Simulation of Population Balance Equation of the Gas Anti-solvent (GAS) Recrystallization Process

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Crystallization process is widely used in various applications such as polymers, dyes, pharmaceuticals, explosives. The new crystallization processes using supercritical fluids have attracted considerable attention because of its environmental advantages by the use of environmentally benign carbon dioxide as a solvent. Gas anti-solvent (GAS) process is one of the most common supercritical processes which utilize the low solubility of the anti-solvent to produce particles. In this work, a mathematical model describing particle size distributions (PSD) of the GAS process is developed and solved numerically. The resulting PSD model is a set of partial differential equations with algebraic constraints, which requires effective numerical approaches. A solution scheme based on the finite element method (FEM) is proposed to solve the dynamic population balance equation using MATLAB. In addition, the population balance equation is also coupled with thermodynamic constraints, rendering conventional FEM methods ineffective. In order to address the issue, we also propose an approximation scheme based on decomposition.