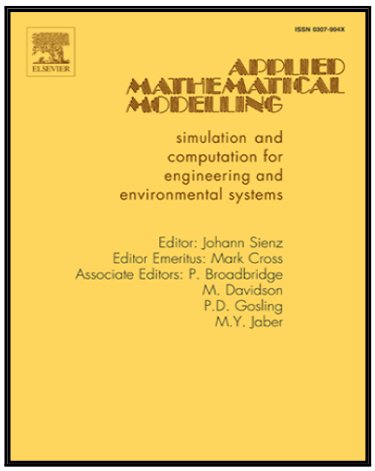

Spectral solution of the breakage–coalescence population balance equation Picard and Newton iteration methods

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Spectral solution of the breakage–coalescence population balance equation Picard and Newton iteration methods

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Abstract

The behavior of dispersed systems such as gas–liquids or liquid–liquid systems depends on the characteristics of the dispersed phase. The population balance (PB) equation is encountered in numerous engineering disciplines in order to describe complex processes where the accurate prediction of the dispersed phase plays a major role for the overall behavior of the system. In the present study, the orthogonal collocation, Galerkin and least-squares methods have been adopted to solve a non-linear PB equation which consists of both breakage and coalescence terms. The performance of the methods is demonstrated by comparing the numerical solution results with the (manufactured) analytical solution of the problem. For the least-squares method, the choice of linearization technique influences the numerical performance, whereas the Galerkin and orthogonal collocation methods obtain the same numerical accuracy for both the Picard and Newton iteration techniques. The least-squares method suffers from lack of convergency using the Picard method. On the other hand, if the Newton method is employed, the least-squares method obtains the same accuracy as the Galerkin and orthogonal collocation methods.

Keywords:

orthogonal collocation; least squares; Galerkin; population balance equation; Picard; Newton method

1 Introduction

The behavior of dispersed systems, such as gas–liquid or liquid–liquid systems, depends strongly on the characteristics of the dispersed phase. Changes in the dispersed phase size and shape distributions may alter the flow pattern severely. The PB equation is encountered in many engineering disciplines, which model complex processes where the accurate prediction of the dispersed phase plays an important role for the overall behavior of the system. Examples of such type of processes can be found in crystallization, bubbly flows, and emulsification systems. In the context of the PB modeling, the dispersed phase can be described in a statistical manner by introducing a density function for the dispersed phase. For example, let $f(\xi,\mathbf{r},t)$ be a number density function where $\mathbf{r}$ is the spatial vector position, ξ denotes the property of interest of the dispersed phase, and t the time. Thus, $f(\xi,\mathbf{r},t)\,\mathrm{d}\xi$ represents the average number of particles per unit volume around the points $\mathbf{r}$ at time t, with the property between ξ and $\xi+\mathrm{d}\xi$. The evolution the density function must take into account the different processes that control the population such as breakage, coalescence, growth and convective transport of the particles. Further details on the PB equation are given elsewhere [1–7].

The numerical solution of PB problems may be computationally intensive [8, 9]. Considerable effort has thus been placed on the development and evaluation of numerical methods for the solution to PB problems [10–13]. The least-squares method has been investigated and applied in the field of solid- and fluid mechanics [14–22]. However, in recent years the least-squares method has been adopted for the solution of chemical reactor problems, e.g. the work of Dorao [23], Zhu [24], Patruno[25], Sporleder[26], and Rout [27]. In the field of chemical reactor engineering, the least-squares method has most frequently been applied to PB problems, but the least-squares method has also been applied for the solution of the pellet equations and fixed packed bed reactor models [28, 29].