Abstract of the Thesis

In this work, new finite volume schemes are proposed for solving one dimensional as well as two dimensional aggregation population balances on non-uniform grids. Moreover, the proposed numerical schemes preserve all the advantages of the conventional discretized methods. The comparison of numerical results obtained by one dimensional new finite volume scheme is shown with the existing schemes for both analytically tractable as well as physically relevant kernels. The results obtained by one dimensional new finite volume scheme for number density and higher order moments are in good agreement with the exact results. However, the higher order moments obtained by finite volume scheme for solving two dimensional aggregation population balance equation show over-prediction with different kernels.

We also present the cell average technique for solving two dimensional aggregation population balance equation on four different regular grids. Numerical results obtained using cell average and fixed pivot techniques on four different types of regular grids are compared with the exact solutions for suitably selected aggregation kernels. The results predicted by the cell average technique are in better agreement with the exact results than the fixed pivot technique. Moreover, the results predicted using the cell average technique on X-type grid with logarithmic scale in the radial direction provide solutions of high quality among all other grids.

Furthermore, we also demonstrate an application of the cell average technique for solving two dimensional population balance equations on irregular triangular grids. It is observed that the main unwanted feature of the triangular mesh is elongated triangles. Strategies for removing such elements are suggested. It is shown that such an improvement reduces the number of pivots by 50% and leads to a drastic reduction of computational time without affecting the accuracy of the solution. Comparison of the numerical solution with the exact solution reveals that the cell average technique on irregular triangular grid produces a better solution in comparison to the cell average technique on a regular triangular grid. It also produces better results in comparison to the fixed pivot technique on both regular triangular and irregular triangular grids. In conclusion, the cell average technique with improved irregular triangular mesh can be seen as the smartest solution technique for the solution of two dimensional population balance equations.

Finally, we also solve backward aggregation population balance equation, i.e., extracting the aggregation laws when the solution of the problem is available. This is well known as 'Inverse Problems'. In this work, we demonstrate a new methodology to obtain the aggregation kernel through the inverse problem approach. This new approach is based on the method of weighted residuals and does not rely on specific traits of the system like self-similarity. The residual approach reduces the inverse problem into solution of a set of linear equations. However, the system of equations is badly conditioned and, therefore, requires regularization for the accurate solution. In this work, Tikhonov regularization technique has been used. The new method has been demonstrated successfully for constant, sum and product kernels.

Keywords: Particulate Processes; Aggregation; Population Balance Equation; Finite Volume Scheme; Regular Grid; Irregular Grid; Inverse Problem; Ill-Posedness; Tikhonov Regularization.