ABSTRACT

In a dynamical system consisting of particles, the spontaneous collision among them results in the change of shape, size, mass etc. of the particles. Thus the particle number density varies with time. In order to incorporate this variation of the particle number density, a mathematical model known as the population balance equation (PBE) is needed. These PBEs are basically a special type of integro-partial differential equations involving linear and non-linear terms depending upon the particulate processes taken into account. In this thesis, we deal with the PBEs corresponding to the coagulation and fragmentation processes. The PBEs representing pure fragmentation is a linear model, whereas, the PBEs representing the coagulation process is non-linear in nature. In these equations, the rate of coagulation and fragmentation are represented through a function called, coagulation kernel and fragmentation kernel, respectively.

In the beginning, we prove the existence of solution of a coagulation fragmentation equation. In this regard, it is necessary to mention that in several industrial phenomenon unwanted formation of dust particles (or particles with nearly zero-mass) take place. So, the system is set up with coagulation kernels having singularity at the axes. Thus the dust particles tend to aggregate at a high rate to form bigger agglomerates. In the literature, a lot of mathematical discussion regarding the existence of solutions considering the non-singular coagulation kernel has been done. So, in this thesis we aim to prove the mathematical existence theory involving the singular coagulation kernel. A generalized form of singular coagulation kernel covering most of the well known singular kernels is tackled using the strong convergence theory. The multiple fragmentation process is chosen, which covers a huge class of unbounded non-singular functions.

While proving the existence of the solutions, it is observed that the exact solution (in closed from) can only be obtained for very particular problems having simple kernels. Therefore, different numerical techniques are applied to find an approximate solution for the complicated problems. In this part of our study we develop a new and efficient numerical scheme approximating the pure fragmentation equa-

tion. The development of this new scheme is based on the finite volume methods and it estimates the particle number density along with the different moments with high accuracy. Furthermore, the new scheme is simple in its mathematical formulation as compared to the other finite volume approximations available in the literature and is robust to apply both on uniform and non-uniform meshes. The development of the new scheme is completed by providing a detailed convergence and consistency analysis of the discrete model. Beside this we compute the new schemes over some test problems to validate the improvement over the previous schemes.

So far, this we have treated one-dimensional PBEs. We now move towards the approximation of multi-dimensional form of the pure fragmentation PBE. It is interesting to mention that only few numerical methods are available in the literature where the multi-dimensional fragmentation equations are approximated. Therefore, we develop a discrete model based on the finite volume methods for solving the multi-dimensional fragmentation equations.

Keywords: Population balance equations; Coagulation; Fragmentation; Existence of solutions; Uniqueness of solutions; Finite volume scheme; Mass conservation; Number preservation; Consistency; Convergence; Multi-dimensional model.