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FINITE VOLUME SCHEME FOR MULTIPLE FRAGMENTATION EQUATIONS

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Abstract. In this paper we study a finite volume approximation for the conservative formulation of multiple fragmentation models. We investigate the convergence of the numerical solutions towards a weak solution of the continuous problem by considering locally bounded kernels. The proof is based on the Dunford-Pettis theorem by using the weak L^1 compactness method. The analysis of the method allows us to prove the convergence of the discretized approximated solution towards a weak solution to the continuous problem in a weighted L^1 space.

Key words. Finite volume, Fragmentation, Convergence, Particle.

1. Introduction

The equations we consider in this paper describe the time evolution of the particle size distribution (PSD) under multiple fragmentation or breakage process. In the simplest equations, each particle is identified by its size, i.e. volume or mass. In multiple breakage, a big particle breaks into two or many fragments. Examples of applications of such models arise in many engineering applications, including aerosol physics, the coalescence and breakup of liquid drops, high shear granulation, crystallization, atmospheric science, highly demanding nano-particles and pharmaceutical industries, see Sommer et al. [16], Gokhale et al. [6] and references therein. Binary breakage is not adequate for some of these applications, therefore, multiple fragmentation is preferred.

The temporal change of the particle number density, $f(t,x) \geq 0$, of particles of volume $x \in \mathbb{R}_{>0}$ at time $t \in \mathbb{R}_{>0}$ in a spatially homogeneous physical system undergoing a breakage process is described by the following well known population balance equation (PBE), see [18]

$$\frac{\partial f(t,x)}{\partial t} = \int_x^\infty b(x,y)S(y)f(t,y)\,dy - S(x)f(t,x), \tag{1}$$

with initial data

$$f(0,x) = f^{in}(x) \geq 0, \quad x \in]0,\infty[. \tag{2}$$

The positive term on the right-hand side describes the creation of particles of size x when a particle of size y breaks. The negative term explains the disappearance of particles of size x into smaller pieces. These terms are known to be the birth and the death term, respectively. The selection rate $S(y)$ gives the rate at which particles of size y are selected to break. The breakage function $b(x,y)$ for a given $y > 0$ gives the size distribution of particle sizes $x \in [0,y[$ resulting from the breakage of a particle of size y. For the particular case of $b(x,y) = 2/y$, the multiple breakage

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turns into the binary breakage PBE. The breakage function satisfies the following important properties

$$\int_0^x b(u,x)du = \bar{N}(x), \quad \int_0^x ub(u,x)du = x. \tag{3}$$

The function $\bar{N}(x)$, which may be infinite, denotes the number of fragments obtained from the breakage of a particle of size x. The second integral shows that the total mass created from the breakage of a particle of size x is again x.

Besides the information given by the evolution of the particle number density distribution, some integral properties like moments are also of great interest in particulate systems. The jth moment of the particle size distribution is defined as

$$\mu_j(t) = \int_0^\infty x^j f(t,x)dx. \tag{4}$$

The first two moments are of special interest. The zeroth ($j = 0$) and first ($j = 1$) moments are proportional to the total number and total mass of particles respectively. Furthermore, the second moment is proportional to the light scattered by particles in the Rayleigh limit [9, p. 1325], [15, p. 267] in some applications. One can easily show that the zeroth moment increases by breakage process while the total mass stays constant. For the total mass conservation, the integral equality

$$\int_0^\infty xf(t,x)\,dx = \int_0^\infty xf^{in}(x)\,dx, \quad t \geq 0,$$

holds.

Several researchers showed the existence of weak solutions for the aggregation-breakage equations with non-increasing mass for a large class of aggregation and fragmentation kernels, see Laurençot [10, 11] and the references therein. Some authors also explained the relationship between discrete and continuous models. For instance, Ziff and McGrady [17] found this relationship for constant and sum breakage kernels while Laurençot and Mischler [11] gave results for the aggregation-breakage models under more general assumptions on the kernels, i.e. for bilinear growth. In the literature, there are various ways to approximate the continuous aggregation-breakage equations including deterministic method [4, 13] and Monte Carlo method [3, 7].

Recently, Bourgade and Filbet [1] have used a finite volume approximation for the binary aggregation-breakage equation. They gave the convergence result of the numerical solutions towards a weak solution of the continuous equation by considering locally bounded kernels. However, their study is restricted to the case of binary breakage. As mentioned above, the case of multiple breakage is of great importance in several applications, especially in high shear granulation. Therefore the aim of this work is to provide a finite volume approximation of the multiple breakage PBE and to investigate its convergence. Though the central idea of this extension is based on the work of Bourgade and Filbet [1], the finite volume approximation and its convergence presented in this work differ due to appearance of completely new kinetics parameters (b and S) in the case of multiple breakage. Following the idea of Bourgade and Filbet, the proof is based on the Dunford-Pettis theorem by using the weak L^1 compactness method and the La Vallée Poussin theorem. We prove