



Development of a mass conserving discretization technique for breakage problems and its convergence analysis

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Abstract In this work an efficient and accurate numerical scheme based on the finite volume method has been introduced to approximate the pure breakage population balance equations. The scheme is designed to conserve the total mass of the particles in the system. The simplicity of both the discrete formulation and its coding are the key features of the new method. It is seen that besides conserving the total mass, the new scheme also gives a better prediction of the total number of the particles in the system as compared to the finite volume scheme of Kumar et al. (Appl Math Comput 219(10):5140–5151, 2013). Unlike [13], the scheme in this paper is computationally very efficient and robust to apply on both the uniform and nonuniform meshes. The development of the new scheme is completed by providing a detailed consistency and convergence analysis of the numerical solution. It is observed that the new scheme is of second order convergent independently of the type of meshes. Moreover, numerical results are compared against several test problems, which include the problems whose solutions are analytically tractable and those which are practically oriented. The mathematical results on convergence analysis of the new scheme has also been verified numerically.

Keywords Population balance equations · Breakage · Finite volume scheme · Consistency · Convergence analysis

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1 Introduction

The dynamical process by which particles undergo changes in their physical properties is called a particulate process. The study of the particulate process is a well known subject in various branches of engineering, physics, chemistry, astrophysics and in many more areas. During the process, spontaneous collisions between the particles cause the changes in their mass, shape, size, volume etc. To study the change of the particle number density $f(x, t) \geq 0$, for particles of volume $x \geq 0$ at time $t \geq 0$ in a physical system undergoing fragmentation process, the following mathematical model known as the *pure breakage population balance equation* (BPBE), is required

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

The Eq. (1) is supplemented by the initial data,

$$f(x, 0) = f_0(x) \geq 0. \quad (2)$$

Without any loss of generality, we consider x and t to be dimensionless quantities [Ref. [24]]. In Eq. (1), $S(x)$ is the selection function and it denotes the rate at which particles of size x are selected to break into smaller fragments. The breakage function $b(x, y)$ is the probability density function denoting the formation of particles of size x due to the breakage of the particles of size y . The breakage function is considered to satisfy the following conditions:

$$\int_0^y b(x, y) dx = v(y), \quad \forall y > 0 \text{ and } b(x, y) = 0, \quad \forall x \geq y \quad (3)$$

and

$$\int_0^y x b(x, y) dx = y, \quad \forall y > 0. \quad (4)$$

The function $v(y)$ in Eq. (3), represents the total number of fragments in which the particle of size y has split during breakage and trivially $v(y) \geq 1$. In general, when a particle of mass y breaks into smaller fragments then the total mass of the fragments formed is equal to y , which has been represented by Eq. (4). For a system which conserves the total mass during fragmentation process, the breakage function $b(x, y)$ is considered to follow Eq. (4).

In the right hand side of Eq. (1), the first term is called the birth term because it denotes the addition of particles of size x in the system due to the breakage of the bigger particle of size y and the second term is called the death term as it removes the particles of size x from the system by breaking them into smaller fragments.

In the literature some authors have dealt with a special form, called the *mass conservative* form of (1). Referring to [13], a mass conservative formulation of the Eq. (1) is written in the following form,

$$\frac{x \partial f(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[\int_x^\infty \int_0^x ub(u, v) S(v) f(v, t) du dv \right], \quad x > 0. \quad (5)$$

The mathematical results on the existence and uniqueness of the solutions of the Eq. (1) in different measure spaces can be found in [3, 17, 18, 21, 22, 25, 28, 29], with suitable bounds over the selection and the breakage functions. But it is seen in the articles [2, 26, 30, 31] that analytical solutions are available only for a limited number of problems with simple forms of selection and breakage functions. In general, the BPBEs with complicated kernels are used widely for various practical experiments. Therefore for those complicated BPBEs, numerical methods are needed to obtain an approximation of the analytical solution.

Besides approximating the number density of the population balance equation, the estimation of its moments are also of great interest in several applications. Moments are mainly the integral properties of the density function and some of them represents physical quantities. Moreover, assessment of different numerical methods usually depend upon their efficiency and accuracy to approximate $f(x, t)$ and its moments. Due to these reasons we formally define the p th moment of the number density function as

$$M_p(t) = \int_0^\infty x^p f(x, t) dx. \quad (6)$$

From the physical point of view, the zeroth moment M_0 and the first moment M_1 are respectively, proportionate to the total number and the total mass of the particles in the system at time t . For the first moment, using the condition (4) it can easily be shown that the following relation is satisfied,

$$\frac{dM_1}{dt} = 0. \quad (7)$$

The Eq. (7) represents mass conservation law of the population balance model represented by Eqs. (1) and (2).

In Eq. (1) we see that the range of the volume variable x varies from 0 to ∞ . To apply a numerical scheme it is necessary to fix a finite range of the computational domain. Let us fix our computational domain as $]0, x_{\max}]$, where $0 < x_{\max} < \infty$. Hence, for $x \in]0, x_{\max}]$ and time $t \in]0, T]$, $T < \infty$, the truncated BPBE takes the following form

$$\frac{\partial f(x, t)}{\partial t} = \int_x^{x_{\max}} b(x, \epsilon) S(\epsilon) f(\epsilon, t) d\epsilon - S(x) f(x, t) \quad (8)$$

with the truncated initial data

$$f(x, 0) = f_0(x) = f^{in}(x) \geq 0, \quad x \in]0, x_{\max}]. \quad (9)$$

Similarly, the limits of the integrals in the Eq. (5) are changed accordingly to obtain the following truncated equation

$$\frac{x \partial f(x, t)}{\partial t} = \frac{\partial}{\partial x} \left[\int_x^{x_{\max}} \int_0^x ub(u, v) S(v) f(v, t) du dv \right], \quad (10)$$

$$x \in]0, x_{\max}].$$

1.1 Existing literatures

In literature the numerical methods like, finite volume methods [4, 5, 10, 13], stochastic methods [19, 23], moment methods [7, 8], sectional methods [9, 16] etc. have been used widely to approximate different forms of the population balance equations (PBEs). With the development of a new numerical scheme it is of great interest for the researchers to study the complete convergence and consistency analysis of that scheme. In this part of the study let us have a review over the literature concerning the development and convergence analysis of the finite volume approximations of the PBEs. To our knowledge, an interesting work in this regard is done by Bourgade and Filbet in [1]. In [1], the authors have proposed a finite volume approximation of the coupled aggregation-binary fragmentation PBEs, in the light of the work of Filbet and Laurençot [4]. Besides, a detailed convergence analysis of the numerical scheme has been provided in [1], where a wide class of aggregation and breakage kernels have been chosen from the space $L_{loc}^\infty(\mathbb{R}^+ \times \mathbb{R}^+)$, $\mathbb{R}^+ = [0, \infty[$. It is to be noted that in both the works [1, 4], the authors have considered the mass conservative formulation of the PBEs. Very recently, Kumar et al. [13] have developed a finite volume scheme approximating the mass conservative form of the pure multiple fragmentation equation (5) and proved the convergence of the approximating solutions. In the article [15], Kumar et al. have developed finite volume

schemes of coupled aggregation-fragmentation equations and in [14] they extended the idea for the PBEs incorporating aggregation, fragmentation, growth and nucleation. Furthermore, a detailed convergence and stability analysis of the scheme proposed in [15] have been provided. It is found in [15], that the order of convergence of the scheme approximating the coupled aggregation-fragmentation equation depends upon the type of meshes, whereas in [13], the scheme approximating the pure BPBE (5), is of second order convergent independently of the meshes.

Other than the above mentioned finite volume approximations of the population balance equations, the convergence analysis of the sectional methods are also available in the literature. In the articles [11, 12], Kumar and Warnecke have done the convergence and stability analysis of the two very well known and efficient numerical schemes, the fixed pivot technique (FPT) and the cell average technique (CAT), approximating the pure multiple fragmentation problems in the form of the Eq. (1). The breakage kernels $S(x)$ and $b(x, y)$ are taken to be twice continuously differentiable functions. It is seen that the convergence rates of FPT and CAT depend upon the different types of meshes. It is also found that on some non-uniform meshes the FPT does not converge whereas the CAT is convergent (of order 1) on those meshes.

The work of Forestier-Coste and Mancini [5] is different from those the previous ones. A numerical approximation of the pure aggregation population balance equation by applying finite volume scheme directly to the Smoluchowski equation has been developed. However, it is found that the developed scheme is unable to conserve the total mass of the system. So, suitable adjustments are made in the scheme so that the modified scheme is able to conserve the total mass of the system. The theory has also been validated numerically by considering different forms of the aggregation kernel.

1.2 State of art

Our work is motivated upon the works of Forestier-Coste and Mancini [5]. In this work a population balance equation having pure multiple fragmentation (1) has been considered. The finite volume method has been applied to approximate the solution of the Eq. (1). But it is seen that the approximated scheme is unable to conserve the total mass of the system. So, suitable changes are made in the discrete scheme to obtain a mass conservative numerical approximation of the truncated equation (8). Furthermore, the completeness of the work has been done by providing a detailed consistency and the convergence analysis of the numerical scheme for the problems whose kernels, $S(x)$ and $b(x, y)$ are twice continuously differentiable functions. All

the mathematical results have been validated numerically for different test problems over different types of locally uniform and non-uniform meshes.

There are many finite volume approximations of the breakage population balance equations available in the literature. So, it is not possible to compare our work with the exhaustive list. Since, the newly developed finite volume scheme in this work approximates the one dimensional BPBEs so we compare the efficiency and novelty of the scheme to the recent finite volume scheme introduced in [13]. For the ease of discussion, let us denote the finite volume scheme of [13] as the *existing finite volume scheme* (EFVS) and the new scheme introduced in this paper as *mass conserving finite volume scheme* (MCFVS). Since, the EFVS has been developed from the mass conservative formulation of the BPBE (5) so both the MCFVS and EFVS are able to conserve the total mass of the system. Compared to EFVS, the additional novelty of the MCFVS is that it provides a better estimation of the total number of particles in the system. It is to be noted that the MCFVS has been developed by applying the finite volume method directly to the multiple breakage equation (1). As a result, MCFVS is simple and hence easy to code whereas owing to the nature of the continuous equation (5), the EFVS is much more complex and so is its coding. Thus from the perspective of computation, simplicity in coding is an additional feature of the MCFVS. In the Sect. 4 several test cases have been considered to observe that MCFVS is much more efficient as it gives a better approximation of the zeroth moment compared to EFVS.

The outline of this paper is as follows. In Sect. 2, the domain has been discretized into small grids and the new finite volume scheme approximating the population balance equation (1) has been developed. Mathematical analysis which includes the consistency and convergence of the newly developed scheme is done in the Sect. 3. Numerical comparison and verification of the mathematical results obtained in the previous sections has been done in Sect. 4 and finally Sect. 5 has been devoted for an overall discussion.

2 The new method

2.1 The discretization method

Let us consider the truncated pure breakage population balance equation (8) along with the initial data (9). We proceed to the discretization procedure firstly, by dividing the continuous computational domain $]0, x_{\max}]$ into a finite $I(< \infty)$ number of subintervals or cells. In this discretization technique we shall approximate the total

number of particles in these I number of subintervals. So, for notational convenience, let us denote those I subintervals as,

$$\Lambda_i :=]x_{i-1/2}, x_{i+1/2}], \quad i = 1, 2, \dots, I,$$

where

$$x_{1/2} = 0, \quad x_{I+1/2} = x_{\max} \quad \text{and} \quad \Delta x_i := x_{i+1/2} - x_{i-1/2}.$$

Let

$$\Delta x = \max_i \Delta x_i, \quad i = 1, 2, \dots, I.$$

The center of each cell Λ_i , i.e., $x_i = \frac{x_{i-1/2} + x_{i+1/2}}{2}$ is referred as the pivot or the grid point of the cell, because it is actually the representative of all size of particles in the cell Λ_i . This type of partitioning of the cell is known as *cell centered* representation of the cell Λ_i .

Let f_i denotes the average value of the number density in the i th cell, i.e.,

$$f_i(t) = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} f(x, t) dx. \tag{11}$$

Assuming sufficient smoothness of the number density $f(x, t)$, by mid-point rule we can have,

$$f_i(t) = f(x_i, t) + \mathcal{O}(\Delta x_i^2). \tag{12}$$

Thus, f_i and $f(x_i, t)$ are same up to the order of Δx^2 . Now, integrating the Eq. (8), over each cell Λ_i gives us a system of equations,

$$\frac{df_i}{dt} = B_i - D_i, \quad i = 1, 2, \dots, I. \tag{13}$$

with the initial data,

$$f_i(0) = f_i^{in} = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} f_0(x) dx, \tag{14}$$

where

$$B_i = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_x^{x_{i+1/2}} b(x, \epsilon) S(\epsilon) f(\epsilon, t) d\epsilon dx \tag{15}$$

and

$$D_i = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} S(x, t) f(x, t) dx. \tag{16}$$

Let \mathbf{f} , \mathbf{f}^{in} , \mathbf{B} , $\mathbf{D} \in \mathbb{R}^I$, are the vectors whose semi-discrete i th components are defined to be f_i , f_i^{in} , B_i and D_i respectively. So, the *semi-discrete* vector form of the Eqs. (13) and (14) is,

$$\left. \begin{aligned} \frac{d\mathbf{f}}{dt} &= \mathbf{B} - \mathbf{D}, \\ \mathbf{f}(0) &= \mathbf{f}^{in}. \end{aligned} \right\} \tag{17}$$

2.2 Formulation of the new scheme

In this part of our study we will develop a new finite volume approximation of the Eq. (13). There are many important numerical schemes available in the literature that has been developed based on the finite volume scheme. But those schemes are developed from the mass conservative formulation of the PBEs. It is of great interest to investigate the scheme that has been developed just by replacing the integrals appearing in the Eq. (13) directly by the quadrature rules. To begin with, we formulate the semi-discrete forms of the birth and the death terms generated due to the application of mid-point quadrature rule to Eq. (13). Let us consider the birth term

$$B_i = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \int_x^{x_{i+1/2}} b(x, \epsilon) S(\epsilon) f(x, t) d\epsilon dx.$$

Changing the order of integration,

$$B_i = \frac{1}{\Delta x_i} \left[\int_{x_{i-1/2}}^{x_{i+1/2}} S(\epsilon) f(\epsilon, t) \int_{x_{i-1/2}}^{\epsilon} b(x, \epsilon) dx d\epsilon + \sum_{k=i+1}^I \int_{x_{k-1/2}}^{x_{k+1/2}} S(\epsilon) f(\epsilon, t) \int_{x_{i-1/2}}^{x_{i+1/2}} b(x, \epsilon) dx d\epsilon \right].$$

Using the *mid-point approximation* for the outer integrals,

$$\begin{aligned} B_i &= S(x_i) f_i \int_{x_{i-1/2}}^{x_i} b(x, x_i) dx + \frac{1}{\Delta x_i} \sum_{k=i+1}^I S(x_k) f_k \Delta x_k \\ &\quad \times \int_{x_{i-1/2}}^{x_{i+1/2}} b(x, x_k) dx + \mathcal{O}(\Delta x^2) \\ &= \frac{1}{\Delta x_i} \sum_{k=i}^I S_k f_k \Delta x_k \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) dx + \mathcal{O}(\Delta x^2), \end{aligned} \tag{18}$$

where

$$p_k^i = \begin{cases} x_i, & \text{when } k = i, \\ x_{i+1/2}, & \text{elsewhere.} \end{cases}$$

The selection function at x_i is denoted by S_i . Similarly, by applying the *mid-point approximation* it can be proved that,

$$D_i = S_i f_i + \mathcal{O}(\Delta x^2). \tag{19}$$

Therefore, using Eqs. (18) and (19) the semi-discrete form of the Eq. (13) obtained by the application of *mid-point quadrature rule* is,

$$\frac{d\hat{f}_i}{dt} = \frac{1}{\Delta x_i} \sum_{k=i}^I S_k \hat{f}_k \Delta x_k \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) dx - S_i \hat{f}_i, \tag{20}$$

along with the initial data

$$\hat{f}_i(0) = f_i(0), \tag{21}$$

where, \hat{f}_i is the numerical approximation of the solution f_i . Hence, the solution of the semi-discrete system (20) and

(21) can be used to approximate the solution of the BPBEs (1) and (2).

It has been already mentioned that the total mass of the system is proportionate to the first moment of the number density function. Therefore, using the analogy with the continuous Eq. (7), a discrete system is said to conserve the total mass if

$$\frac{d}{dt} \left(\sum_{i=1}^I x_i \hat{f}_i \Delta x_i \right) = 0. \tag{22}$$

However, in the following theorem, it will be observed that the proposed discrete formulation (20) fails to conserve the total mass of the system.

Theorem 2.1 The discrete formulation (20) does not conserve the total volume or mass; that is,

$$\frac{d}{dt} \sum_{i=1}^I (x_i \hat{f}_i \Delta x_i) \neq 0. \tag{23}$$

Proof Let us multiply x_i on both sides of the formulation (20) and then summing over i we obtain

$$\begin{aligned} \frac{d}{dt} \sum_{i=1}^I (x_i \hat{f}_i \Delta x_i) &= \sum_{i=1}^I x_i \sum_{k=i}^I S_k \hat{f}_k \Delta x_k \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) dx \\ &\quad - \sum_{i=1}^I x_i S_i \hat{f}_i \Delta x_i \end{aligned} \tag{24}$$

Changing the order of the sums and using the fact that $\int_0^{x_k} x b(x, x_k) dx = x_k$ we get,

$$\begin{aligned} \frac{d}{dt} \sum_{i=1}^I (x_i \hat{f}_i \Delta x_i) &= \sum_{k=1}^I S_k \hat{f}_k \Delta x_k \sum_{i=1}^k x_i \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) dx \\ &\quad - \sum_{i=1}^I x_i S_i \hat{f}_i \Delta x_i \\ &= \sum_{k=1}^I S_k \hat{f}_k \Delta x_k \left[\sum_{i=1}^k x_i \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) dx - x_k \right] \\ &= \sum_{k=1}^I S_k \hat{f}_k \Delta x_k \left[\sum_{i=1}^k x_i \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) dx \right. \\ &\quad \left. - \sum_{i=1}^k \int_{x_{i-1/2}}^{p_k^i} x b(x, x_k) dx \right] \\ &= \sum_{k=1}^I S_k \hat{f}_k \Delta x_k \left[\sum_{i=1}^k \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) (x_i - x) dx \right] \\ &\neq 0. \end{aligned} \tag{25}$$

This proves the assertion (23) of the Theorem 2.1. \square

However for a particulate system, besides approximating the number density function it is also utmost necessary that the numerical scheme conserves the total

mass of the system. Since the discrete formulation (20) fails to conserve the total mass of the particulate system so it can not be a suitable method to approximate (1). This drawback leads us to develop a new numerical scheme which conserve the total mass of the system. This new scheme is developed by certain appropriate changes in the death terms of the relation (20) such that it satisfies the mass conservation laws. So, using the particle number density approximations the discrete formulation of the new *mass conserving finite volume scheme* (MCFVS) is given by,

$$\frac{d\hat{f}_i}{dt} = \frac{1}{\Delta x_i} \sum_{k=i}^I S_k \hat{f}_k \Delta x_k \int_{x_{i-1/2}}^{p_k^i} b(x, x_k) dx - \omega_i S_i \hat{f}_i \tag{26}$$

The weight ω_i has been introduced so that the scheme can conserve the total mass of the particles in the system, i.e., it satisfies Eq. (22). To get the value of ω_i for which the formulation (26) satisfies the mass conservation law we prove the following theorem.

Theorem 2.2 The discrete formulation (26) conserves the total mass if

$$\omega_i = \frac{\sum_{j=1}^i x_j \int_{x_{j-1/2}}^{p_j^i} b(x, x_i) dx}{x_i}. \tag{27}$$

Proof Starting with the Eq. (26) and proceeding in the similar manner as done in the proof of Theorem 2.1 and using (27), we will easily get that

$$\frac{d}{dt} \sum_{i=1}^I (x_i \hat{f}_i \Delta x_i) = 0.$$

Hence, the assertion is proved. \square

Remark 2.1 The weight ω_i is independent of the number density function and the breakage function has been assumed to be constant in time, therefore it can be calculated prior to the computation of the system of differential equations (26). But in general, the breakage function is time dependent. In that case, the weights have to be calculated at each time step of the computation

For this new numerical scheme let the modified approximated birth and death terms in each of the i th cell are written as \hat{B}_i and \hat{D}_i respectively. So, writing Eq. (26) in terms of \hat{B}_i and \hat{D}_i ,

$$\frac{d\hat{f}_i}{dt} = \hat{B}_i - \hat{D}_i, \quad i = 1, 2, \dots, I, \tag{28}$$

along with the initial condition

$$\hat{f}_i(0) = f_i(0), \tag{29}$$

where,

$$\hat{B}_i := \frac{1}{\Delta x_i} \sum_{k=i}^I S_k \hat{f}_k \Delta x_k \int_{x_{i-1/2}}^{x_i} b(x, x_k) dx \tag{30}$$

and

$$\hat{D}_i := \omega_i S_i \hat{f}_i. \tag{31}$$

Let us denote the vector $\hat{\mathbf{f}} = [\hat{f}_1, \hat{f}_2, \dots, \hat{f}_I]$. Therefore, the formulation (28) and (29) take the following spatially discretized vector form in \mathbb{R}^I

$$\left. \begin{aligned} \frac{d\hat{\mathbf{f}}}{dt} &= \hat{\mathbf{B}}(\hat{\mathbf{f}}) - \hat{\mathbf{D}}(\hat{\mathbf{f}}) =: \mathbf{J}(\hat{\mathbf{f}}), \\ \hat{\mathbf{f}}(0) &= \mathbf{f}^{in} \end{aligned} \right\} \tag{32}$$

where $\hat{\mathbf{B}}, \hat{\mathbf{D}} \in \mathbb{R}^I$ are the functions of $\hat{\mathbf{f}}$ whose i th components are $\hat{B}_i(\hat{\mathbf{f}})$ and $\hat{D}_i(\hat{\mathbf{f}})$ respectively and $\mathbf{J}(\hat{\mathbf{f}}) = [J_1(\hat{f}_1), J_2(\hat{f}_2), \dots, J_I(\hat{f}_I)]$.

3 Convergence analysis

Before we proceed to check the consistency and convergence of the semi-discrete system (32), let us first gather some useful theorems and definitions from Hundsdorfer and Verwer [6] and Linz [20], which will be used in this part of the study. Let the discrete L^1 norm on \mathbb{R}^I be defined as

$$\|\mathbf{f}(t)\| = \sum_{i=1}^I |f_i(t)| \Delta x_i. \tag{33}$$

Let $\mathbf{J}(\mathbf{f})$ is the vector function obtained by replacing $\hat{\mathbf{f}}$ with \mathbf{f} in the relation (32).

Definition 3.1 The spatial truncation error is defined by the residual left by substituting the exact solution $\mathbf{f} = [f_1(t), f_2(t), \dots, f_I(t)]$ in to the equation as

$$\boldsymbol{\sigma}(t) = \frac{d\mathbf{f}(t)}{dt} - \mathbf{J}(\mathbf{f}). \tag{34}$$

The scheme is called consistent of order p if, for $\Delta x \rightarrow 0$ $\|\boldsymbol{\sigma}(t)\| = \mathcal{O}(\Delta x^p)$, uniformly for all $t, 0 \leq t \leq T$. $\tag{35}$

Definition 3.2 The global discretization error is defined by $\boldsymbol{\epsilon}(t) = \mathbf{f}(t) - \hat{\mathbf{f}}(t)$. The scheme is called to be convergent of order p if, for $\Delta x \rightarrow 0$,

$$\|\boldsymbol{\epsilon}(t)\| = \mathcal{O}(\Delta x^p), \text{ uniformly for all } t, 0 \leq t \leq T. \tag{36}$$

It is important that our numerical solution remains non-negative for all t . Let us write $\mathbf{M} \geq 0$ for a vector $\mathbf{M} \in \mathbb{R}^I$ if and only if all its components are non-negative.

Theorem 3.1 Suppose that $\mathbf{J}(\mathbf{f})$ is continuous and satisfies the Lipschitz condition

$$\|\mathbf{J}(\mathbf{f}) - \mathbf{J}(\mathbf{g})\| \leq L \|\mathbf{f} - \mathbf{g}\|, \text{ for all } \mathbf{f}, \mathbf{g} \in \mathbb{R}^I, L < \infty.$$

Then the solution of the semi-discrete system (32) is non-negative if and only if for any vector $\mathbf{f} \in \mathbb{R}^I$ and all $i = 1, 2, \dots, I$ and $t \geq 0$,

$$\mathbf{f} \geq 0, \quad f_i = 0 \Rightarrow J_i(\mathbf{f}) \geq 0.$$

Proof The proof of this theorem is given in Hundsdorfer & Verwer [6], Theorem 7.1, Chapter 1. \square

Theorem 3.2 Let us assume that a Lipschitz condition on $\mathbf{J}(\mathbf{f})$ is satisfied for $0 \leq t \leq T$ and for all $\mathbf{f}, \hat{\mathbf{f}} \in \mathbb{R}^I$, i.e., there exists a Lipschitz constant $L < \infty$ such that

$$\|\mathbf{J}(\mathbf{f}) - \mathbf{J}(\hat{\mathbf{f}})\| \leq L \|\mathbf{f} - \hat{\mathbf{f}}\|, \text{ for all } \mathbf{f}, \hat{\mathbf{f}} \in \mathbb{R}^I \tag{37}$$

holds. Then a consistent discretization method is also convergent and the convergence order is the same as the order of the consistency.

Proof The proof of a generalized version of the above theorem have been provided in Linz [20]. \square

This is the most important theorem of this article. If we can show that $\mathbf{J}(\hat{\mathbf{f}})$ satisfies Lipschitz condition and the system (32) is consistent, then by the direct application of the Theorem 3.2 we will get the convergence of the scheme. Moreover, the convergence order will be the same of the order of the consistency.

In the following theorem we proceed to check under what conditions the function $\mathbf{J}(\mathbf{f})$ satisfies Lipschitz condition (37).

Theorem 3.3 Let us assume that S and b are twice continuously differentiable functions over $]0, x_{\max}]$ and $]0, x_{\max}] \times]0, x_{\max}]$, respectively. Then, for all $\mathbf{f}, \hat{\mathbf{f}} \in \mathbb{R}^I$, there exists a $L = 2 \max_{x \in]0, x_{\max}] } [S(x)v(x) < \infty$, independent of Δx , such that the Lipschitz condition over $\mathbf{J}(\hat{\mathbf{f}})$, i.e.,

$$\|\mathbf{J}(\mathbf{f}) - \mathbf{J}(\hat{\mathbf{f}})\| \leq L \|\mathbf{f} - \hat{\mathbf{f}}\|,$$

holds good.

Proof Let us first denote

$$b_{i,k} := \int_{x_{i-1/2}}^{x_i} b(x, x_k) dx.$$

Therefore,

$$\begin{aligned} \|\mathbf{J}(\mathbf{f}) - \mathbf{J}(\hat{\mathbf{f}})\| &= \sum_{i=1}^I |J_i(f_i) - J_i(\hat{f}_i)| \Delta x_i \\ &= \sum_{i=1}^I \frac{1}{\Delta x_i} \left| \sum_{k=i}^I S_k b_{i,k} (f_k - \hat{f}_k) \Delta x_k - \omega_i S_i (f_i - \hat{f}_i) \Delta x_i \right| \Delta x_i \\ &\leq \sum_{i=1}^I \sum_{k=i}^I S_k b_{i,k} |f_k - \hat{f}_k| \Delta x_k + \sum_{i=1}^I \omega_i S_i |f_i - \hat{f}_i| \Delta x_i \end{aligned} \tag{38}$$

For $j \leq i$, implies $x_j \leq x_i$ for all $j = 1, 2, \dots, i$ and so using it in (27)

$$\omega_i = \frac{\sum_{j=1}^i x_j b_{j,i}}{x_i} \leq \frac{x_i \sum_{j=1}^i b_{j,i}}{x_i} = v(x_i). \tag{39}$$

Therefore, using the inequality (39) in the r.h.s. of the relation (38), we get

$$\begin{aligned} \|\mathbf{J}(\mathbf{f}) - \mathbf{J}(\hat{\mathbf{f}})\| &\leq \sum_{i=1}^I \sum_{k=1}^I S_k b_{i,k} |f_k - \hat{f}_k| \Delta x_k \\ &\quad + \sum_{i=1}^I v(x_i) S_i |f_i - \hat{f}_i| \Delta x_i. \end{aligned} \tag{40}$$

Changing the order of the sums in the first term of (40)

$$\begin{aligned} \|\mathbf{J}(\mathbf{f}) - \mathbf{J}(\hat{\mathbf{f}})\| &\leq \sum_{k=1}^I \left[S_k |f_k - \hat{f}_k| \Delta x_k \sum_{i=1}^k b_{i,k} \right] \\ &\quad + \sum_{i=1}^I v(x_i) S_i |f_i - \hat{f}_i| \Delta x_i \\ &= \sum_{k=1}^I S_k v(x_k) |f_k - \hat{f}_k| \Delta x_k \\ &\quad + \sum_{i=1}^I v(x_i) S_i |f_i - \hat{f}_i| \Delta x_i \\ &= 2 \sum_{k=1}^I S_k v(x_k) |f_k - \hat{f}_k| \Delta x_k \\ &\leq 2 \sum_{k=1}^I \left(\max_k [S_k v(x_k)] \right) |f_k - \hat{f}_k| \Delta x_k \\ &\leq 2 \max_{x \in]0, x_{\max}[} [S(x)v(x)] \|\mathbf{f} - \hat{\mathbf{f}}\| \\ &\leq L \|\mathbf{f} - \hat{\mathbf{f}}\|. \end{aligned} \tag{41}$$

where $L = 2 \max_{x \in]0, x_{\max}[} [S(x)v(x)] < \infty$, the Lipschitz constant independent of Δx . Hence, the function $\mathbf{J}(\mathbf{f})$ satisfies the Lipschitz criterion. \square

Let us now proceed to check whether the scheme (32) is consistent or not.

3.1 Consistency and convergence

The following theorem is stated and proved to obtain the order of consistency of the MCFVS (32) for the pure breakage population balance equations.

Theorem 3.4 Consider the functions S and b are twice continuously differentiable functions over $]0, x_{\max}[$ and $]0, x_{\max}[\times]0, x_{\max}[$, respectively. Then for any family of meshes, the solution of the semi-discrete system (32) is non-negative and second order consistent. Moreover, the method is convergent and the order of convergence is the same as the order of consistency.

Proof Non-negativity: For any non-negative vector $\hat{\mathbf{f}} \in \mathbb{R}^I$ whose i th component is zero, i.e., for any $\hat{\mathbf{f}} \in \mathbb{R}^I$ with $\hat{\mathbf{f}} \geq 0$ and $\hat{f}_i = 0$, the relations (30) and (31) give

$$\hat{B}_i(\hat{\mathbf{f}}) \geq 0 \quad \text{and} \quad \hat{D}_i(\hat{\mathbf{f}}) = 0.$$

Hence, $J_i(\hat{\mathbf{f}}) \geq 0$ for all $i = 1, 2, \dots, I$. Now, applying the Theorem 3.1 and Theorem 3.3, we get the non-negativity of the solution $\hat{\mathbf{f}}$.

Consistency: By the definition 3.1 the spatial truncation error over each of the i th cell is given by

$$\sigma_i(t) = \frac{df_i(t)}{dt} - J_i(f_i(t)) \tag{42}$$

Using the expressions (15), (16), (30) and (31) in the right hand side of the Eq. (42) we get,

$$\begin{aligned} \frac{df_i(t)}{dt} - J_i(f_i(t)) &= (B_i - D_i) - (\hat{B}_i(\mathbf{f}) - \hat{D}_i(\mathbf{f})) \\ &= (B_i - \hat{B}_i(\mathbf{f})) - (D_i - \hat{D}_i(\mathbf{f})) \end{aligned} \tag{43}$$

Now we deal with the terms $(B_i - \hat{B}_i(\mathbf{f}))$ and $(D_i - \hat{D}_i(\mathbf{f}))$ separately. By using the relation (18) and (30), we get

$$(B_i - \hat{B}_i(\mathbf{f})) = \mathcal{O}(\Delta x^2). \tag{44}$$

Now for the death term from the relations (19) and (31), we get,

$$(D_i - \hat{D}_i(\mathbf{f})) = (1 - \omega_i) S_i f_i + \mathcal{O}(\Delta x^2). \tag{45}$$

Then

$$\begin{aligned} 1 - \omega_i &= \frac{1}{x_i} \left[x_i - \sum_{j=1}^i x_j b_{j,i} \right] \\ &= \frac{1}{x_i} \left[\int_0^{x_i} x b(x, x_i) dx - \sum_{j=1}^i x_j b_{j,i} \right] \\ &= \frac{1}{x_i} \sum_{j=1}^i \int_{x_{j-1/2}}^{x_j} (x - x_j) b(x, x_i) dx \\ &= \frac{1}{x_i} \left[\sum_{j=1}^{i-1} \int_{x_{j-1/2}}^{x_{j+1/2}} (x - x_j) b(x, x_i) dx \right. \\ &\quad \left. + \int_{x_{i-1/2}}^{x_i} (x - x_i) b(x, x_i) dx \right]. \end{aligned} \tag{46}$$

With the application of the mid-point approximation for $j = 1, 2, \dots, i - 1$ and right-end approximation for $j = i$ we obtain that the numerator of (46) is of $\mathcal{O}(\Delta x^2)$.

Hence, we have

$$1 - \omega_i = \mathcal{O}(\Delta x^2) \quad i = 1, 2, \dots, I. \tag{47}$$

Using the relation (47) in the Eq. (45), we get

$$(D_i - \hat{D}_i(\mathbf{f})) = \mathcal{O}(\Delta x^2). \tag{48}$$

Therefore, combining both the cases (44) and (48), we get

$$\sigma_i(t) = \mathcal{O}(\Delta x^2).$$

Hence, the order of consistency of the *mass-conserving discrete* scheme (32), for pure breakage process is obtained as

$$\|\sigma(t)\| = \sum_{i=1}^I |\sigma_i(t)| \Delta x_i = \mathcal{O}(\Delta x^2), \quad (49)$$

and this order is independent of the type of meshes or intervals.

Convergence: Combining Theorem 3.2, Theorem 3.3 and the above result on consistency the convergence of the proposed method is proved. Moreover, Theorem 3.1 implies that the order of convergence is same as the order of consistency, i.e., 2. \square

Remark 3.1 From the work of Dobovskii and Stewart [3], it can be followed that the smoothness of the kernels S and b implies the smoothness of the solution function f . In this work the functions S and b are considered to be twice continuously differentiable and so the solution function f .

4 Numerical comparison

In this section, we verify the results obtained in Sects. 2 and 3 numerically, i.e., we verify how efficiently the proposed numerical scheme MCFVS estimates the particle number density and its two moments (zeroth and first) and also find the experimental (numerical) order of convergence (EOC). The numerical verifications are based on applying the MCFVS (32) to several test problems over different types of meshes. Let $[x_{\min}, x_{\max}]$ be the computational domain. In order to show that the order of convergence of MCFVS is independent of the type of meshes, we consider both *non-uniform* and *locally uniform* type of meshes (Ref. [13]).

Due to the nature of formation of the non-uniform meshes we have taken $x_{\min} = 10^{-9}$ and $x_{\max} = 1$ throughout this work. The dimensionless values of the all the concerned quantities have been considered during computation. The dimensionless breakage extent provided in the paper is obtained by dividing the zeroth moment of the density function by the initial zeroth moment, i.e., $M_0(t)/M_0(0)$ at the final time of computation. Similarly, in order to make the particle number density and its first moment dimensionless, normalization of those properties are done by dividing their values at different times by their initial values. A comparison of the normalized first and the zeroth moment obtained by MCFVS and the EFVS ([13]) has been presented here. The numerical values of EOC and relative error of the scheme are calculated as in Kumar and Warnecke [11, 12].

Three different test problems have been considered for numerical comparison and verification of the mathematical results. In the first case, a test problem having an exact solution is taken. The solution can be found in [26, 31]. Since, the exact solution is available we plot the numerical results of particle number density function, the first and the zeroth moment against the exact results. The second and the third case are more practical oriented problems with complicated breakage functions and initial conditions. The problems in the test cases II and III, do not possess the exact solutions. So, in the second and third cases the number density function cannot be plotted for comparison. For solving the discrete system (32), MATLAB ODE45 solver is used.

4.1 Test case I

Let us consider a problem with binary breakage function $b(x, y) = \frac{2}{y}$ and the quadratic selection function $S(x) = x^2$. Let the number density satisfies the mono-dispersed initial condition, i.e.,

$$f(x, 0) = \delta(x - 1) = \begin{cases} 0, & \text{when } 0 \leq x < 1, \\ 1, & \text{when } x = 1. \end{cases}$$

The computation is carried out by dividing the domain into 30 initial sub-intervals and at time $t = 50$. The breakage extent is obtained as $\frac{M_0(t)}{M_0(0)} \approx 8$.

The Fig. 1 represents the prediction of the particle number density and its first and the zeroth moments against their exact values. In Fig. 1a, the particle number density is plotted against the representative of the respective meshes. It is seen that the overall prediction of the particle number density is pretty good. In the Fig. 1b the numerical result of the first and the zeroth moment is compared with the exact value. It is observed that both the MCFVS and EFVS conserve the first moment but the numerical results of the zeroth moment is better when approximated using MCFVS.

In the Table 1, the relative error along with the EOC have been calculated for the locally uniform meshes (Table 1a) and the non-uniform meshes (Table 1b). In both the cases numerical values up to 480 grid points have been provided. From both the tables, it is observed that the experimental order of convergence is approximately 2 and it is independent of the type of meshes.

4.2 Test case II

In this case, we consider a complicated breakage function

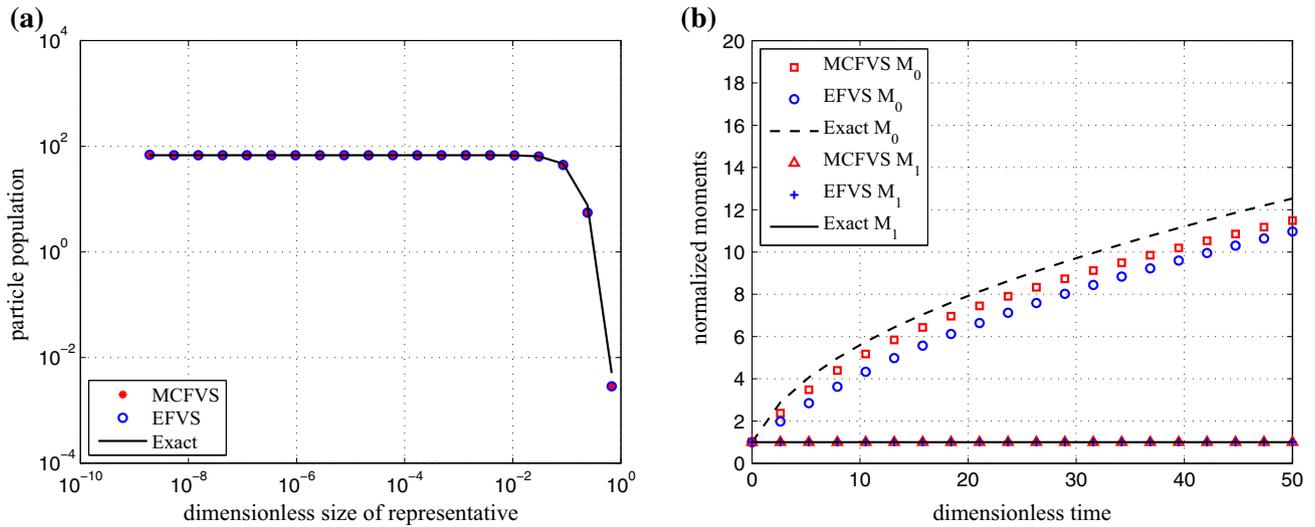


Fig. 1 Exact and numerical values of the particle number density (left) and the normalized first and the zeroth moments (right) for test case I

Table 1 EOC of the numerical scheme MCFVS for Test case I

Grid points	Relative error L_1	EOC
(a) Locally uniform meshes		
30	0.0301	–
60	0.0083	1.8633
120	0.0021	1.9586
240	0.0005	1.9891
480	0.0001	1.9972
(b) Non-uniform meshes		
30	0.0083	–
60	0.0021	1.9586
120	0.0005	1.9891
240	0.0001	1.9972
480	3.1E-5	1.9994

$$b(x, y) = \frac{p x^c (y - x)^{c+(c+1)(p-2)} [c + (c + 1)(p - 1)]!}{y^{c+(c+1)(p-1)} [c]! [c + (c + 1)(p - 2)]!}, \tag{50}$$

which is used considerably for various experimental purposes. As defined in [13, 27], the parameters p and c of (50) denote the number of fragments and shape factor respectively. Here, by setting $p = 4, c = 2$ and $p = 8, c = 2$ we consider two multi-fragmentation problems. Let us also consider the linear selection function, $S(x) = x$ and the initial condition to satisfy the following normal distribution

$$f(x, 0) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x - \mu)^2}{2\sigma^2}\right]$$

where, $\sigma^2 = 0.01, \mu = 0.5$. The computations are carried out for 60 initial grids and at time $t = 50$. For $p = 4, c = 2$

and $p = 8, c = 2$ the approximate breakage extents obtained are 76 and 176, respectively. The exact solution of this problem is not available in the literature. Therefore, we are not able to compare exact and the numerical values of the particle number density function. But due to the linear selection function we are able to plot the exact values of the zeroth and the first moments. In the Fig. 2, the numerical values of the moments have been compared against the exact values. From the Fig. 2a and b, it is seen that both the schemes conserve the total mass of the system but MCFVS gives a better prediction of the total number of the particles in the system.

The relative error and the EOC of the proposed scheme MCFVS have been shown in Tables 2 and 3. As desired the EOC of the MCFVS is approximately 2 and is independent of the type of the meshes.

4.3 Test case III

In this case we consider two test problems almost similar to the problems that has been considered in Test case II, but with a quadratic selection function, $S(x) = x^2$. The breakage functions and the initial conditions are same as considered in the previous case. The solution of this problem is also not available in the literature. Due to the quadratic selection function we can not find the exact values of the moments. So, only the relative error and the EOC of the MCFVS have been represented in the Tables 4 and 5. The computations are done for 60 initial grids and $t = 50$. The approximate breakage extent obtained is 11 for $p = 4, c = 2$ and 19 when $p = 8, c = 2$.

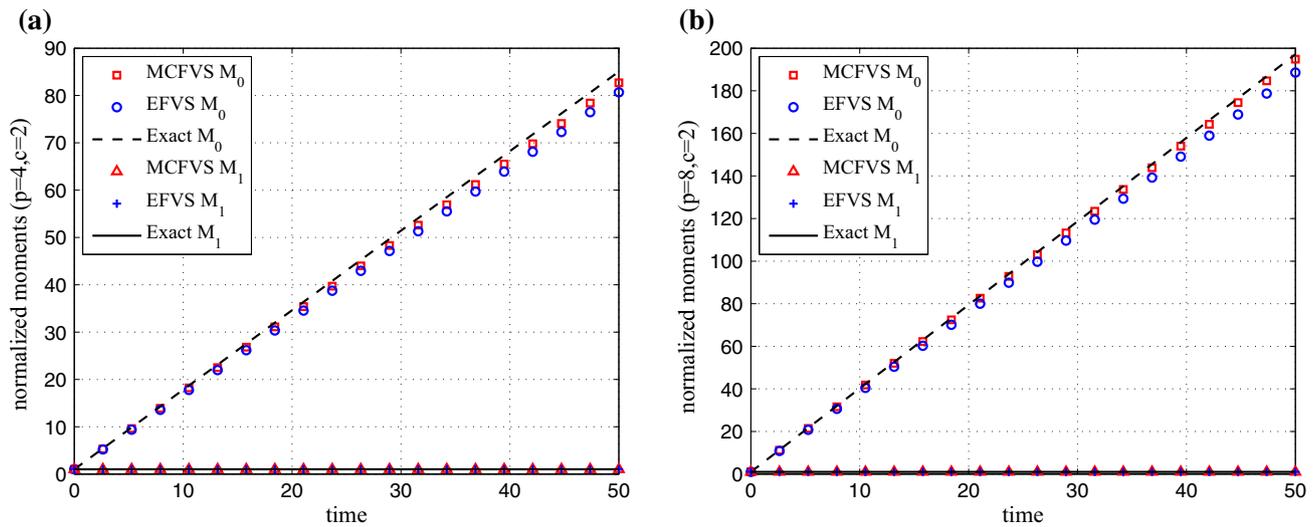


Fig. 2 Comparison of the numerical and exact values of the moments for test case II

Table 2 EOC of the numerical scheme MCFVS for $p = 4, c = 2$ (Test case II)

Grid points	Relative error L_1	EOC
(a) Locally uniform meshes		
60	–	–
120	1.2942	–
240	0.2916	2.1499
480	0.0711	2.0353
960	0.0177	2.0078
(b) Non-uniform meshes		
60	–	–
120	0.9159	–
240	0.1834	2.3203
480	0.0455	2.0097
960	0.0114	2.0009

Table 3 EOC of the numerical scheme MCFVS for $p = 8, c = 2$ (Test case II)

Grid points	Relative error L_1	EOC
(a) Locally uniform meshes		
60	–	–
120	3.5039	–
240	0.8023	2.1266
480	0.1973	2.0236
960	0.0491	2.0056
(b) Non-uniform meshes		
60	–	–
120	2.6103	–
240	0.5533	2.2379
480	0.1378	2.0051
960	0.0344	2.0000

Table 4 EOC of the numerical scheme MCFVS for $p = 4, c = 2$ (Test case III)

Grid points	Relative error L_1	EOC
(a) Locally uniform meshes		
60	–	–
120	0.2458	–
240	0.0572	2.1042
480	0.0140	2.0263
960	0.0035	2.0041
(b) Non-uniform meshes		
60	–	–
120	0.1841	–
240	0.0391	2.2371
480	0.0097	1.9995
960	0.0024	2.0003

Table 5 EOC of the numerical scheme MCFVS for $p = 8, c = 2$ (Test case III)

Grid points	Relative error L_1	EOC
(a) Locally uniform meshes		
60	–	–
120	0.5592	–
240	0.1289	2.1171
480	0.0318	2.0184
960	0.0079	2.0042
(b) Non-uniform meshes		
60	–	–
120	0.4231	–
240	0.0934	2.1788
480	0.0234	1.9973
960	0.0058	1.9992

From the Tables 4 and 5 it is seen that the MCFVS is second order convergent and is independent of the type of meshes.

5 Results and discussion

A new numerical method MCFVS has been developed for the pure multiple breakage population balance equation (1) using the finite volume approximation. Besides predicting the particle number density well, the scheme also conserves the total mass of the particles and gives a better estimation of the total number of particles in the system as compared to the most recent finite volume approximation of the BPBEs [13]. Furthermore, MCFVS is simple scheme and easy to code. A complete mathematical analysis by checking the consistency of the error bounds and the order of convergence of the MCFVS has been done. It is observed that the proposed numerical scheme is second order convergent and this rate is independent of the type of the grids or meshes. The theoretical observations have been validated with different test cases of numerical examples. The examples of simple problems whose solutions are tractable and complex practically oriented problems which do not have solutions have been considered.

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