1. Introduction

Population balances is a classical approach to describe the changes that take place in the various particulate systems. Major applications of particulate processes are in the area of pharmaceutical where sprayed fluidized bed granulator [15], twin-screw wet granulator [19] etc. are used to prepare granules. In these processes, the properties of the particles such as size, shape, porosity etc. vary due to aggregation, breakage, growth and nucleation mechanisms. In the pharmaceutical industry, multiple particle properties are required to describe the quality of the granules [16]. So, in this work, the problem related to the 2D pure aggregation population balance equation is solved. Aggregation (or agglomeration) is a complex formation mechanism in which larger sized particles are formed due to the merging of two or more smaller size particles. During this mechanism, the total number of particles decreases gradually with time but the total mass of the system remains the same.

Mathematically, the aggregation mechanism is expressed in terms of a non-linear integro-partial differential equation [14,30] which is used to track the change in number of particles in the system. During this mechanism, the number of particles (or number density) can vary to several order of magnitude and can acquire a sharp peak. Therefore, to track the true behavior of number density, an accurate and efficient numerical scheme is required. In literature, many authors developed various numerical schemes including finite difference methods [34], finite element methods [1,3,18], monte carlo method [27–29], method of moments [42,43], least-square spectral method [9], finite volume schemes [12,17,20,33,37,40], direct quadrature method of moments [2,8,10,26,32] or sectional methods like the fixed pivot technique (FPT) [22,25,41] and cell average technique (CAT) [5,21,23,24,38].

Among all these existing techniques, sectional methods are known for their ability to predict the number distribution as well as various order moments accurately. The major disadvantage of the sectional methods is that their mathematical formulations are very complex, making the computations very expensive whereas the finite volume schemes are well known for their simple mathematical formulations. But the finite volume schemes were not able to predict the higher order moments with significant accuracy [12,33]. However, two finite volume schemes were recently developed by Singh et al. [35] and Kaur et al. [17] which not only predict the number distribution accurately but also higher order moments with some certain accuracy. Still, the accuracy of the higher order moments can be improved by choosing an appropriate discretization as shown by sectional methods when implemented on various grids [4,7,31,35]. This significantly shows that the
orientation and directionality of the grid plays significant role in predicting the various results accurately. However, the applications of the finite volume scheme are only limited to rectangular and triangular grids [36]. The triangular grid is generated by the slicing rectangular grid along the diagonal as shown in Fig. 1. Therefore, in this work, the effect of the directionality and orientation of the grids (discretizations) on the solution of a 2D PBE is analyzed by treating four different discretizations with a mass conserving finite volume scheme.

The paper is ordered as follows: Section 2 provides the mathematical model required to describe the 2D aggregation mechanism. Next section is used to express the idea of the generation of four different types of triangular grids and the implementation of the finite volume scheme on these grids. Further, Section 4 is devoted to conduct a comparison of numerical results computed using different grids with the exact results for analytically relevant kernels. In final section, conclusions and remarks of this work are made.

2. Mathematical model

This section is used to describe the mathematical model required to track the changes takes place in the number density function \( n(x, y, t) \) as various size particles are formed in the system due to the aggregation process. Therefore, a 2D pure agglomeration population balance equation (PBE) in a well-mixed system can be written as follows:

\[
\frac{\partial n(x, y, t)}{\partial t} = 1 \int x' \int y' K(x-x', y-y', x', y') n(x-x', y-y', t) n(x', y', t) dx' dy' - \int x_0 \int y_0 K(x, y, x', y') n(x, y, t) n(x', y', t) dx' dy'
\]

with initial data

\[
n(x, y, 0) = n_0(x, y), x \in [0, \infty].
\]

Here the aggregation kernel \( K(x, y, x', y', t) \) interpret the successive collision of the two smaller size particles to build a larger size particle. Mathematical structure of the aggregation kernel is \( K(x, y, x', y', t) = K_0(t) K'(x, y, x', y', t) \) where the prefactor \( K_0(t) \) describes the efficiency of the collision. Moreover, the aggregation kernel is non-negative and symmetric with respect to size variables. For the simplicity, the size dependent (or time independent) kernels are considered for this study, i.e., \( K_0(t) = 1 \). The most common examples of time independent kernels are \( K'(x, y, x', y', t) = 1 + y + x + y' + x'y' \). The schematic demonstration of the aggregation process is given in Fig. 2.

Since the PBE (1) is chosen to be solved with numerical method, but due to the presence of infinity in the second integral, it is very difficult to solve numerically. Hence, for the implementation of the numerical scheme, the domain must be restricted to

\[
\lambda=\{(x, y): 0 < x < x_{\text{max}}, 0 < y < y_{\text{max}}\}.
\]

Therefore, the eq. (1) takes the following form

\[
\frac{\partial n(x, y, t)}{\partial t} = \int x' \int y' K(x-x', y-y', x', y') n(x-x', y-y', t) n(x', y', t) dx' dy' - \int x' \int y' K(x, y, x', y') n(x, y, t) n(x', y', t) dx' dy'
\]

with initial condition changes to

\[
n(x, y, 0) = n_0(x, y), x \in [0, x_{\text{max}}], y \in [0, y_{\text{max}}].
\]

Further to understand the complete behavior of the system, other than number density function some integral properties namely moments of the distribution are also required [15,39]. The \( j \)th moment of the number density function \( n(x, y, t) \) is defined by

\[
\mu_j(t) = \int_0^\infty \int_0^\infty x^j y^n n(x, y, t) dx dy
\]

Here, the zeroth order moment \( \mu_0 \) represents the total number of particles in the system. Whereas \( \mu_{10} \) and \( \mu_{01} \) expresses the total mass of the particles along the x and y axes, respectively. Moreover, the summation of \( \mu_{10} \) and \( \mu_{01} \) describes the total mass of the particles in the system.

3. Numerical discretizations

In this section, the mathematical formulation of the finite volume scheme on a non-uniform regular triangular grid for solving 2D aggregation PBE (2) is presented. Before providing the expressions of the numerical scheme, we first provide the brief description of the generation of four type of non-uniform regular triangular grids. The MATLAB commands voronoi and delaunayTriangulation are used to create the voronoi region and triangulation, respectively for all discretizations.
3.1. Types of domain discretizations

For generating the different grids, it is essential to fix the lower and upper bounds of the discretization domain along the horizontal axis (x-axis) and vertical axis (y-axis) as $x_{1/2} = y_{1/2} = 0$ and $[0, x_{\text{max}}]$ and $[0, y_{\text{max}}]$, respectively with $x_{\text{max}}, y_{\text{max}} < \infty$. Further, let us denote $i$ and $j$ as the two indices which is associated with $R^{th}$ cell along $x$ and $y$ directions, respectively where $R = \{p_1, p_2, \ldots, p_i\}$ for $I$ number of cells. The lower and upper boundaries of the $P^{th}$ cell are denoted by $(x_{i-1/2}, y_{j-1/2})$ and $(x_{i+1/2}, y_{j+1/2})$, respectively, for $i = 1, 2, \ldots, I_1$ and $j = 1, 2, \ldots, I_2$. Here, the scalar values $I_1$, $I_2$ are the number of divisions of the domain in $x$ and $y$ directions, respectively. Therefore the total number of cells obtained are $I = I_1 \times I_2$. Corresponding to these boundaries, the ‘representative’ of the cell can be obtained as follows:

$$x_i = \frac{x_{i-1/2} + x_{i+1/2}}{2}, \quad y_j = \frac{y_{j-1/2} + y_{j+1/2}}{2},$$

and the length of the $P$ th cell along $m$ and $n$ directions is defined as

$$\Delta x_i = x_{i+1/2} - x_{i-1/2}, \quad \Delta y_j = y_{j+1/2} - y_{j-1/2}.$$

respectively.
Type-1 discretization

Draw 16 lines with exponentially increasing distance between the lines along both horizontal and vertical axes. The points at which both axes cut each other are known as grid points (lower & upper boundaries) of cells. The points on both axes are uniformly drawn on a logarithmic scale. Therefore, a larger number of grid points are obtained near the origin of the grid and decreases as we move towards the end of the grid. Further adopting these grid points, Voronoi partitioning and Delaunay triangulation is completed. We name this grid as Type-1 discretization and its representation can be seen in Fig. 3(a).

Type-2 discretization

This discretization is generated using two types of lines: (a) radial r-lines and (b) perpendicular t-lines are considered. The r-lines are those lines which pass through the origin and equally partition the domain space. In our case, we have considered 16 radial lines with the angle between any two consecutive lines is \( \frac{90}{23} = 3.91^\circ \). The t-lines are the lines of slope \( -1 \). We have considered 16 t-lines for discretization. The grid points are formed when r-lines and t-lines are intersecting. The total number of pivots obtained is \( 15 \times 15 = 225 \). Every pivot is representing some Voronoi region. Similar to the previous discretization, using these pivots, Delaunay triangulation is performed to form triangular elements. We call this discretization as Type-2 or X-type discretization. It can be noticed from the Fig. 3(b) that pivots are heavily located near the origin whereas the pivot’s density reduces as we move far from the origin.

Type-3 Discretization

This grid is generating by modifying the previous grid (see Section3.1.2). In contrast to the previous grid, the r-lines and t-lines are drawn on a logarithmic scale along both axes (see Fig. 3(c)). Moreover, the angles between two consecutive t-lines are considered in a way that these angles increases exponentially towards the center of the plane. This implies that the angle between lines lies near axes is smaller as compared to the angles between lines lies in the center of the grid. Whereas, the r-lines are drawn with exponentially increasing distance between the lines. In this case, 16 r-lines and 16 t-lines are considered which obtained in total 225 grid points and the points at which both lines cut each other are called pivots which are associated to some Voronoi region. Using these pivots, the triangular elements are formed. Analogous to previous grids, the more grid points are densely packed

### Table 1

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_{\text{min}}, y_{\text{min}} )</td>
<td>( 10^{-4} )</td>
</tr>
<tr>
<td>( x_{\text{max}}, y_{\text{max}} )</td>
<td>20</td>
</tr>
<tr>
<td>Initial time</td>
<td>0</td>
</tr>
<tr>
<td>Final time</td>
<td>35</td>
</tr>
<tr>
<td>( I_{\text{agg}} )</td>
<td>0.97</td>
</tr>
<tr>
<td>( x_{\text{agg}}, y_{\text{agg}} )</td>
<td>1</td>
</tr>
<tr>
<td>( N_0 )</td>
<td>1</td>
</tr>
<tr>
<td>Number of cells</td>
<td>( 15 \times 15 )</td>
</tr>
</tbody>
</table>
near the origin of the domain and lesser at the end of the domain. We call this grid as Type-3 discretization.

### 3.1.4. Type-4 Discretization

This grid was first proposed by Nandanwar and Kumar [31] which consist of circular arcs (c-arcs) and radial lines (r-lines). The idea of this grid is to overcome the shortcomings due to the random orientation of triangles. To generate this grid, the radial lines are drawn in a way that the angles between any two adjacent lines remain same whereas the circular arcs are drawn in a logarithmic scale. The circular arcs are densely packed near the origin and it exponentially increases as we move far from the origin. The intersection points of these r-lines and c-arcs are considered to be the grid points. Similar to the previous cases, the formation of cells and triangles is completed. We call this grid as Type-4 discretization and can be seen in 3(b).

In this work, we have considered 16 r-lines and 16 c-arcs, producing 225 pivots. Note: Similar kind of study was also conducted by Singh et al. [35] with the cell average technique (CAT) to solve the 2D aggregation PBE. The major drawback is that the distribution of particles to neighboring pivots after the aggregation is required in the cell average technique Kumar et al. [21]. Therefore, large number of grid points are required to capture the accurate solutions of various moments and number distribution functions with these discretizations. In particular, 23 × 25(=575) grid points were used to generate all four discretizations which makes the simulations computationally very expensive. However, in our study, we only consider 225 number of cells because no distribution of particles is required for the finite volume scheme.

Now based on the aforementioned notions, let us introduce the mathematical expression of the finite volume scheme for a non-uniform regular triangular grid.

### 3.2. Finite volume scheme

This section is devoted to describe the mathematical formulation of the finite volume scheme developed by Singh et al. [40] for solving a bivariate aggregation PBE on a non-uniform regular triangular grid. Before describing the numerical scheme, let us presume that $N_{m_p, n_q}$ expresses the number of particles in the cell having representatives $P = (x_i, y_j)$ which can be calculated mathematically by integrating the number density function ($n(x, y, t)$) over the boundaries of the cell, i.e.,

$$N_{x_i, y_j} = \int_{x_i - 1/2}^{x_i + 1/2} \int_{y_j - 1/2}^{y_j + 1/2} n(x, y, t) dx dy.$$  \hspace{1cm} (4)

Additionally, it is also assumed that the particles present within cells are concentrated on the representatives of each cell so that Dirac delta point masses can be used to approximate the number density function,
i.e.,

\[ n(x, y, t) = \sum_{i=1}^{l_1} \sum_{j=1}^{l_2} N_{x,i,j} \delta(x-x_i) \delta(y-y_j). \]  

(5)

Substituting the Eq. (5) in the PBE (2) and integrate over the variables \(x\) and \(y\) will give the following expression:

\[
\frac{dN_{x,y}}{dt} = B_{x,y} - D_{x,y},
\]

(6)

where the terms \(B_{x,y}\) and \(D_{x,y}\) describes the birth and death of the particles in the \(ij\)th cell, respectively and are given by

\[
B_{x,y} = \sum_{p,q}^{l_1,l_2} \sum_{r,s}^{l_1,l_2} \left( 1 - \frac{1}{2} \delta_{p,q} \delta_{r,s} \right) K_{p,q,r,s} N_{x,p,q} N_{y,r,s},
\]

(7)

and

\[
D_{x,y} = \sum_{p=1}^{l_1} \sum_{q=1}^{l_2} K_{p,q,r,s} N_{x,p,q} N_{r,s},
\]

(8)

Here \(K_{p,q,r,s} = K_{x_p,y_q,x_r,y_s}\) is used for simplicity. The detailed derivation of above equations is provided in Kumar et al. [21]. Moreover, it can be observed that the formulation represented by the Eq. (6) captures the number preservation property very well, however, it does not conserve the total mass of the system which is a necessary condition for any finite volume scheme (see Appendix A). This can be easily achieved by adding a weight to the formulation (6) which yields

\[
\frac{dN_{x,y}}{dt} = \sum_{(p,q,r,s) \in \Omega^{ij}} \left( 1 - \frac{1}{2} \delta_{p,q} \delta_{r,s} \right) K_{p,q,r,s} N_{x,p,q} N_{y,r,s} \Lambda_{p,q,r,s}^{ij}
\]

- \[
\sum_{p=1}^{l_1} \sum_{q=1}^{l_2} K_{p,q,r,s} N_{x,p,q} N_{r,s},
\]

(9)

Here the weight is defined by

\[
\Lambda_{p,q,r,s}^{ij} = \begin{cases} 
\frac{x_p + x_q + y_r + y_s}{x_r + y_j}, & (p, q, r, s) \in \Omega^{ij} \\
0, & \text{otherwise}.
\end{cases}
\]

(10)

Here, \(\Lambda_{p,q,r,s}^{ij}\) is responsible for the conservation of the mass of the system. Moreover, \(\Omega^{ij}\) is defined as a pair of cells having representative \((x_p, y_q)\) and \((x_r, y_s)\) such that after the aggregation, i.e., \((x_p + x_q + y_r + y_s)\) falls in a cell having representative \((x_j, y_j)\) and mathematically can be...
Fig. 7. Different order moments and number density using size-independent kernel with Type-4 discretization.

<table>
<thead>
<tr>
<th>( \psi )</th>
<th>Type-1</th>
<th>Type-2</th>
<th>Type-3</th>
<th>Type-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \psi_{00} )</td>
<td>0.36142</td>
<td>0.18080</td>
<td>0.59055</td>
<td>0.24997</td>
</tr>
<tr>
<td>( \psi_{10} )</td>
<td>0.36142</td>
<td>0.18080</td>
<td>0.59055</td>
<td>0.24997</td>
</tr>
<tr>
<td>( \psi_{20} )</td>
<td>0.36142</td>
<td>0.18080</td>
<td>0.59055</td>
<td>0.24997</td>
</tr>
<tr>
<td>( \psi_{11} )</td>
<td>0.40433</td>
<td>0.13099</td>
<td>0.56943</td>
<td>0.14138</td>
</tr>
<tr>
<td>( \psi_{21} )</td>
<td>0.53061</td>
<td>0.17481</td>
<td>0.63832</td>
<td>0.18252</td>
</tr>
</tbody>
</table>

Table 3
Weighted error of number distribution using size-independent kernel with various grids (15 × 15).

<table>
<thead>
<tr>
<th>( \psi )</th>
<th>Type-1</th>
<th>Type-2</th>
<th>Type-3</th>
<th>Type-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \psi_{00} )</td>
<td>0.21423</td>
<td>0.05896</td>
<td>0.29523</td>
<td>0.13311</td>
</tr>
<tr>
<td>( \psi_{10} )</td>
<td>0.21423</td>
<td>0.05896</td>
<td>0.29523</td>
<td>0.13311</td>
</tr>
<tr>
<td>( \psi_{20} )</td>
<td>0.21423</td>
<td>0.05896</td>
<td>0.29523</td>
<td>0.13311</td>
</tr>
<tr>
<td>( \psi_{11} )</td>
<td>0.28433</td>
<td>0.04267</td>
<td>0.31763</td>
<td>0.06058</td>
</tr>
<tr>
<td>( \psi_{21} )</td>
<td>0.29265</td>
<td>0.06729</td>
<td>0.30897</td>
<td>0.08345</td>
</tr>
<tr>
<td>( \psi_{30} )</td>
<td>0.21423</td>
<td>0.05896</td>
<td>0.29523</td>
<td>0.13311</td>
</tr>
</tbody>
</table>

Table 5
Maximum error in different order moments using size-independent kernel with 15 × 15 cells.

<table>
<thead>
<tr>
<th>( \eta )</th>
<th>Type-1</th>
<th>Type-2</th>
<th>Type-3</th>
<th>Type-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \eta_{00} )</td>
<td>0.12367</td>
<td>0.08311</td>
<td>0.09421</td>
<td>0.10974</td>
</tr>
<tr>
<td>( \eta_{10} )</td>
<td>3.39 × 10^{-7}</td>
<td>4.25 × 10^{-9}</td>
<td>1.32 × 10^{-6}</td>
<td>8.66 × 10^{-6}</td>
</tr>
<tr>
<td>( \eta_{20} )</td>
<td>0.17949</td>
<td>0.00849</td>
<td>0.11415</td>
<td>0.04764</td>
</tr>
<tr>
<td>( \eta_{11} )</td>
<td>0.24662</td>
<td>0.02071</td>
<td>0.24030</td>
<td>0.05011</td>
</tr>
<tr>
<td>( \eta_{21} )</td>
<td>0.41981</td>
<td>0.02432</td>
<td>0.38496</td>
<td>0.02721</td>
</tr>
<tr>
<td>( \eta_{30} )</td>
<td>0.56396</td>
<td>0.26336</td>
<td>0.35669</td>
<td>0.29488</td>
</tr>
</tbody>
</table>

Table 4
Maximum error in different order moments using size-independent kernel with 30 × 30 cells.

<table>
<thead>
<tr>
<th>( \eta )</th>
<th>Type-1</th>
<th>Type-2</th>
<th>Type-3</th>
<th>Type-4</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \eta_{00} )</td>
<td>0.08956</td>
<td>0.02625</td>
<td>0.06652</td>
<td>0.04595</td>
</tr>
<tr>
<td>( \eta_{10} )</td>
<td>2.21 × 10^{-11}</td>
<td>1.91 × 10^{-15}</td>
<td>9.16 × 10^{-10}</td>
<td>4.89 × 10^{-10}</td>
</tr>
<tr>
<td>( \eta_{20} )</td>
<td>0.09657</td>
<td>0.00219</td>
<td>0.05942</td>
<td>0.01324</td>
</tr>
<tr>
<td>( \eta_{11} )</td>
<td>0.14778</td>
<td>0.00932</td>
<td>0.13091</td>
<td>0.03957</td>
</tr>
<tr>
<td>( \eta_{21} )</td>
<td>0.23378</td>
<td>0.01056</td>
<td>0.20524</td>
<td>0.01591</td>
</tr>
<tr>
<td>( \eta_{30} )</td>
<td>0.29657</td>
<td>0.11978</td>
<td>0.21986</td>
<td>0.16533</td>
</tr>
</tbody>
</table>
Further, integrate the Eq. (9) with respect to time from limits \( t_k \) to \( t_{k+1} \), we get the final relation for the finite volume scheme as

\[
N_{x,y}^{k+1} = N_{x,y}^{k} + \Delta t \left( \sum_{l=1}^{1} \beta_{l} \delta_{y} \delta_{y} x_{l} y_{l} \sum_{p=1}^{P} K_{l} \phi_{l}, x_{l}, y_{l}, x_{l}, y_{l} \right)
\]

where \( \Delta t = t_{k+1} - t_{k} \) for \( k \in \{0,1,...,N-1\} \). The detailed description of the finite volume scheme and the theoretical proof of the mass conservation property along with the CFL condition for the positivity of the solution can be found in Singh et al. [40].

### 4. Results and discussion

In this part of the paper, the numerical results determined using FVS with various triangular discretizations are compared with the analytical results for different analytically relevant kernels. Gelbard and Seinfeld [13] and Fernández-Díaz and Gómez-García (2007) have provided the analytical solutions for size-independent and size-dependent kernels, respectively corresponding to the distinct initial conditions. For our study, the initial condition \( n(x,y,0) = \frac{100}{x^{6/2} y^{6/2}} \exp\left(-\frac{2x}{\Delta x} - \frac{2y}{\Delta y}\right) \) is chosen for calculating the numerical as well as analytical (or exact) solutions. The comparison is conducted in terms of various order moments along with the particle population in each cell, i.e., the number density functions. Simulations are run using MATLAB on a i5 CPU with 2.40 GHz and 8 GB RAM.

Since the number density function will be 3D surface plot (i.e., \( n(x,y,t) \) vs \( x \) vs \( y \)) and to see the difference between analytical and numerical solutions is very difficult in a single plot. Therefore, the concept of flat representation suggested by Chakraborty and Kumar [4] is used. In the flat representation, cells are sorted from \( \Delta t \) to \( \Delta t+1 \), we get the final relation for the finite volume scheme as

\[
N_{x,y}^{k+1} = N_{x,y}^{k} + \Delta t \left( \sum_{l=1}^{P} K_{l} \phi_{l}, x_{l}, y_{l}, x_{l}, y_{l} \right)
\]

where \( \Delta t = t_{k+1} - t_{k} \) for \( k \in \{0,1,...,N-1\} \). The detailed description of the finite volume scheme and the theoretical proof of the mass conservation property along with the CFL condition for the positivity of the solution can be found in Singh et al. [40].

### 4. Results and discussion

In this part of the paper, the numerical results determined using FVS with various triangular discretizations are compared with the analytical results for different analytically relevant kernels. Gelbard and Seinfeld [13] and Fernández-Díaz and Gómez-García (2007) have provided the analytical solutions for size-independent and size-dependent kernels, respectively corresponding to the distinct initial conditions. For our study, the initial condition \( n(x,y,0) = \frac{100}{x^{6/2} y^{6/2}} \exp\left(-\frac{2x}{\Delta x} - \frac{2y}{\Delta y}\right) \) is chosen for calculating the numerical as well as analytical (or exact) solutions. The comparison is conducted in terms of various order moments along with the particle population in each cell, i.e., the number density functions. Simulations are run using MATLAB on a i5 CPU with 2.40 GHz and 8 GB RAM.

Since the number density function will be 3D surface plot (i.e., \( n(x,y,t) \) vs \( x \) vs \( y \)) and to see the difference between analytical and numerical solutions is very difficult in a single plot. Therefore, the concept of flat representation suggested by Chakraborty and Kumar [4] is used. In the flat representation, cells are sorted from \( \Delta t \) to \( \Delta t+1 \), we get the final relation for the finite volume scheme as

\[
N_{x,y}^{k+1} = N_{x,y}^{k} + \Delta t \left( \sum_{l=1}^{P} K_{l} \phi_{l}, x_{l}, y_{l}, x_{l}, y_{l} \right)
\]

where \( \Delta t = t_{k+1} - t_{k} \) for \( k \in \{0,1,...,N-1\} \). The detailed description of the finite volume scheme and the theoretical proof of the mass conservation property along with the CFL condition for the positivity of the solution can be found in Singh et al. [40].

### 4. Results and discussion

In this part of the paper, the numerical results determined using FVS with various triangular discretizations are compared with the analytical results for different analytically relevant kernels. Gelbard and Seinfeld [13] and Fernández-Díaz and Gómez-García (2007) have provided the analytical solutions for size-independent and size-dependent kernels, respectively corresponding to the distinct initial conditions. For our study, the initial condition \( n(x,y,0) = \frac{100}{x^{6/2} y^{6/2}} \exp\left(-\frac{2x}{\Delta x} - \frac{2y}{\Delta y}\right) \) is chosen for calculating the numerical as well as analytical (or exact) solutions. The comparison is conducted in terms of various order moments along with the particle population in each cell, i.e., the number density functions. Simulations are run using MATLAB on a i5 CPU with 2.40 GHz and 8 GB RAM.

Since the number density function will be 3D surface plot (i.e., \( n(x,y,t) \) vs \( x \) vs \( y \)) and to see the difference between analytical and numerical solutions is very difficult in a single plot. Therefore, the concept of flat representation suggested by Chakraborty and Kumar [4] is used. In the flat representation, cells are sorted from \( \Delta t \) to \( \Delta t+1 \), we get the final relation for the finite volume scheme as

\[
N_{x,y}^{k+1} = N_{x,y}^{k} + \Delta t \left( \sum_{l=1}^{P} K_{l} \phi_{l}, x_{l}, y_{l}, x_{l}, y_{l} \right)
\]

where \( \Delta t = t_{k+1} - t_{k} \) for \( k \in \{0,1,...,N-1\} \). The detailed description of the finite volume scheme and the theoretical proof of the mass conservation property along with the CFL condition for the positivity of the solution can be found in Singh et al. [40].
The symbols $\text{exc}$ and $\text{num}$ represent the exact and numerical solutions, respectively. Moreover, $\psi_{00}$ and $\psi_{10}$ or $\psi_{01}$ expresses the relative error in the total number of particles (zeroth order moment) and the total mass of the system (first order moments), respectively over the whole domain. Similarly, other combinations of $i$ and $j$ can be computed. Additionally, the maximum error in various order moments are calculated using the mathematical expression

$$\eta_{ij} = \max_t \left| \frac{\mu_{ij}^{\text{exc}}(t) - \mu_{ij}^{\text{num}}(t)}{\mu_{ij}^{\text{exc}}(t)} \right|.$$  

Here $\eta_{00}$ and $\eta_{10}$ exhibits the maximum errors in the zeroth and first order moments, respectively. These errors are evaluated at the final time.

Before interpreting the different numerical result, it is necessary to define degree of aggregation (DOA) $I_{\text{agg}}$:

$$I_{\text{agg}}(t) = 1 - \frac{\mu_{00}(t)}{\mu_{00}(t=0)}, \quad t \geq 0.$$  

which describes the reduction of number of initial primary particles due to agglomeration process. Initially at $t = 0$, $I_{\text{agg}} = 0$ and as the limit $t$ approaches $\infty$, $I_{\text{agg}}$ tends to unity with all primary particles forming one aggregate.

4.1. Size-independent Kernel

Firstly, a size-independent kernel, i.e., $K(t,x,y,x',y') = K_0(t)$ is chosen to conduct the comparison of numerical and analytical results. This kernel is also well known as an constant kernel. For simplicity, the value of $K_0(t) = 1$ which physically reveals that the aggregation between two particles will always take place when they collide with each other. Other parameters required to run a simulation for a size-independent aggregation kernel are listed in Table 1. The analytical result for the number density function was derived by Gelbard and Seinfeld [13].

The quantitative comparison of various order moments and number density functions corresponding to four various discretizations are illustrated in Figs. 4, 5, 6 and 7. It can be observed that the zeroth order moments which denotes the number of particles in each cell predicted numerically show over prediction from the analytical result. This is possibly due to the fact that this numerical scheme is only focused on conserving the total mass of the system rather than preserving the zeroth order moment. Moreover, the total mass of the system, i.e., the first order moments obtained numerically using all discretization are matching well with the analytical result. In addition, the second order moments ($\mu_{20}$ & $\mu_{11}$) computed numerically are showing a more accurate solution for Type-2 discretization than the other three discretizations. Moreover, similar kind of behavior is exhibited by the third order moments, i.e., the third order moment approximated with Type-2 discretization shows lesser deviation from the analytical moment than the other grids.
Analogous to above qualitative analysis, we have also analyzed the results related to the number density functions graphically as shown in Figs. 4(d), 5(d), 6(d) and 7(d) using the notion of flat representation for four different discretizations. The results reveal that the particle population in each cell (number density function) computed for the Type-2 discretization shows better approximation than the other grids. This same conclusion can also be made when quantitative weighted sectional errors (13) in number density functions for four discretizations are calculated (see Table 2). It can be observed that the weighted sectional errors in various order moments obtained using Type-2 discretization is comparatively lesser than the other discretizations. Furthermore, the total maximum errors exist in various order moments are quantified using the expression (14) in Table 4 for four distinct discretizations. One can notice that the maximum errors in different order moments computed using Type-1, Type-3 and Type-4 are more as compared to the errors calculated using Type-2 grid. Moreover, the same comparison is also conducted using a refined grid with cell $30 \times 30$ as shown in Tables 3 and 5. It can be observed that the quantitative sectional and maximum errors reduced significantly for each discretizations when calculated using a refined grid. However, still Type-2 discretization performs better than the other discretizations.

In order to show the efficiency of the finite volume scheme with various discretizations, the comparison of various grids is also conducted in terms of computational time, i.e., the time taken by the finite volume scheme to obtain the various numerical results. Table 6 demonstrates that the computational time taken for computing all numerical results by Type-2 is lesser than the other discretizations. Hence, from the above discussion, it can be easily concluded that the finite volume scheme with the Type-2 discretization computes the different results more accurately and efficiently than the other three discretizations.

4.2. Size-dependent Kernel

Similar to the previous kernel, the numerical simulations are also run for obtaining the results corresponding to the size-dependent kernel, i.e., $K(x, y, x', y', t) = K_0(t)(x + y + x' + y')$ where $K_0(t) = 1$. This is also known as an additive kernel. In contrast to the size-independent kernel, the larger size particles aggregate at a faster rate for this kernel due to higher size dependency of the kernel. The analytical result for the number density function using this complex kernel was derived by [11]. The parameters required to run the simulation for this kernel are listed in Table 7.

The numerical results for various order moments along with the number density function predicted using the finite volume scheme with four discretizations are demonstrated in Figs. 8, 9, 10 and 11. It can be observed that the zeroth order moments obtained using Type-1, Type-3 and Type-4 discretizations show over-prediction from the analytical result whereas the zeroth order moment predicted with Type-2 matches well with the analytical moment. Additionally, the first order moments for four kinds of discretizations show very good agreement with the analytical result, i.e., the mass conservation property holds for all discretizations. Moreover, the second order moments $\langle \mu \rangle_1$ &
predicted using Type-2 discretization shows less deviation from the analytical moment whereas the moments computed using the other three discretizations show significant deviation (under prediction) from the analytical moment. Likewise, the third order moments ($\mu_{21}$ & $\mu_{30}$) also show the similar behavior as second order moments, i.e., the moments predicted by Type-1, Type-3 and Type-4 deviate far from the analytical solutions whereas the third order moments captured using Type-2 show less deviation from the analytical moments.

Analogous to the previous case, for the size-dependent kernel, the number density function obtained numerically for various discretizations are compared graphically (see Figs. 8(d), 9(d), 10(d) and 11(d)). For analyzing the number density functions, the concept of at representation is used. Figs reveal that Type-2 discretization approximates the number density function with higher precision as compared to the other discretizations. The quantitative weighted sectional errors in the number density function calculated using the relation (13) are listed in Table 8 for all discretizations. The results exhibit that the errors exist in Type-2 are lesser as compared to Type-1, Type-3 and Type-4 discretizations. In addition, the maximum errors (14) in various order moments obtained using finite volume scheme with four discretizations are also demonstrated in Table 10. The results reveal that the maximum errors computed at the end of time domain are lesser for Type-2 discretization as compared to the other grids. In order to check the accuracy of the finite volume scheme on a refined grid, the quantitative comparison of sectional and maximum errors exist in various order moments is also conducted in Tables 9 and 11. It can be noticed that these errors reduce to 50% when finite volume scheme is implemented on a refined grid for each discretization. However, the Type-2 discretization still outperforms the other discretizations in term of accuracy.

In addition to above, the comparison in terms of computational sense shows that slightly lesser time is taken by finite volume scheme with the Type-2 grid than the other three discretizations. Therefore, it can be concluded that the finite volume scheme with Type-2 discretization approximates the various order moments as well as number density function with higher accuracy and efficiency as compared to the other grids. This also illustrates that the solution of the 2D aggregation PBE is highly dependent on the type of discretization chosen to divide the given domain.

5. Conclusions

The finite volume scheme has been applied successfully to four types of non-uniform regular triangular discretizations. Different comparisons of the finite volume scheme with four types of discretizations in terms of maximum as well as sectional weighted errors have been conducted. The qualitative along with the quantitative numerical results computed using the finite volume scheme admit that the results approximated for Type-2 discretization are in better agreement with the analytical results as compared to the results of all other grids. This concludes that the finite volume scheme for solving a 2D aggregation population balance equation is highly dependent on the orientation and
directionality of discretization considered for partitioning the given domain.

Appendix A. Appendix

Proposition: The numerical scheme representing by the expression (6) is not mass conserving.

Proof: Multiply the formulation provided in eq. (6) by \((x_i + y_j)\) both side and take sum over all \(i\) and \(j\). The left hand side gives the first moment at time \(t^{k+1}\) and the right hand side can be simplified as

\[
\sum_{i=1}^{l_1} \sum_{j=1}^{l_2} N_{i,j}^{k+1} (x_i + y_j) \Delta x_i \Delta y_j = \sum_{i=1}^{l_1} \sum_{j=1}^{l_2} N_{i,j}^{k+1} (x_i + y_j) \Delta x_i \Delta y_j + \Delta t \Delta T,
\]

where \(T\) is given by the following expression:

\[
T = \sum_{i=1}^{l_1} \sum_{j=1}^{l_2} \left( \sum_{p,q,r,s} \left( 1 - \frac{1}{2} \theta_{pq} \theta_{rs} \right) N_{p,q,r,s}^{k+1} N_{i,j}^{k+1} N_{p,q} N_{r,s} - \sum_{p=1}^{l_1} \sum_{q=1}^{l_2} \left( \frac{1}{2} \theta_{pq} \theta_{rs} \right) N_{p,q}^{k+1} N_{i,j}^{k+1} N_{p,q} \right)
\]

For proving the mass conservation property, it is required to show that \(T = 0\) for all times. But, it can be noticed that the two expressions on the right hand side of the above equations are not same. Hence, the mass conservation property does not hold for the formulation (6).

References


Nomenclature

Symbol: Description
n: Number distribution (density) function
K: Aggregation kernel
K_{agg}(t): Aggregation frequency
M \psi(t)^{\text{Iagg}}(\lambda): Analytical (Exact) value of number of particles in the cell p at time t
M \psi(t)^{\text{num}}(\lambda): Numerical value of number of particles in the cell p at time t
\mu: Moments of number density function
\mu: Total number of cells
\mu: Degree of aggregation
\lambda: Restricted domain
\eta: Particle properties in terms of size (volume)
A: Weight for the finite volume scheme
\psi: Weighted sectional errors in number density function
\gamma: Maximum errors in moments

Abbreviations
PBE: Population balance equation
FVS: Finite volume scheme
CAT: Cell average technique
DOA: Degree of aggregation