

# Extension of moment projection method to the fragmentation process

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## Abstract

The method of moments is a simple but efficient method of solving the population balance equation which describes particle dynamics. Recently, the moment projection method (MPM) was proposed and validated for particle inception, coagulation, growth and, more importantly, shrinkage; here the method is extended to include the fragmentation process. The performance of MPM is tested for 13 different test cases for different fragmentation kernels, fragment distribution functions and initial conditions. Comparisons are made with the quadrature method of moments (QMOM), hybrid method of moments (HMOM) and a high-precision stochastic solution calculated using the established direct simulation algorithm (DSA) and advantages of MPM are drawn.

*Keywords:* Fragmentation, breakage, method of moments, population balance, moment projection method, particulate systems

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## 1. Introduction

Fragmentation (also referred to as breakage) is a process by which particles break into two or more fragments leading to an increase in the number of particles [1]. For this reason it plays an important role in a number of chemical processes [2]. In fluidised-bed combustion, the rate of fragmentation during particle burnout influences the overall burning rate of single coal particles [3]. Arguably, in practical combustion systems, predicting particle destruction can be as important as predicting particle formation and growth. It is found in Ref. [4] that the inclusion of fragmentation improved model predictions of soot particle size distributions (PSDs) from a diesel engine.

The evolution of the PSD with time is described by the population balance equation (PBE) with mechanisms which modify the particles such as inception, coagulation (otherwise known as aggregation), growth, and shrinkage where particles reduce in mass and are eventually removed from the system [5–7]. In Ref. [8] the PBE for a particulate system undergoing fragmentation is studied and it is found that the PSD obeys a first-order linear ordinary integro-differential equation. The complexity of the equation depends on the fragmentation kernel and fragment distribution function, and analytical solutions only exist for certain restrictive cases.

A number of methods have been proposed to solve these types of equations which can be broadly classified as: method of moments (MOM) (see, e.g., Refs. [2, 4–7, 9–21]), sectional method (see, e.g., Refs. [1, 9, 22–29]) and stochastic method (see, e.g., Refs. [11, 30–35]). These methods often encompass a trade-off between physical detail and computational efficiency. In the stochastic method the particle population is represented by an en-

semble of stochastic particles and the particle processes are treated probabilistically [36]. The stochastic solution has been proven to converge to the deterministic solution of the PBE [33]. The method easily allows a highly detailed particle description; however, under certain conditions, the computational time [34] and memory requirement [35] can be intractable. Sectional methods divide the mass range into a finite number of sections [24]. The PSD within each section evolves according to an ordinary differential equation which can be solved by standard solvers (see, e.g., Refs. [25–28]). The computational time rapidly scales with the number of internal coordinates tracked and the number of sections required to achieve convergence [29].

When the PBE is written in terms of one or two internal coordinates, MOM is a particularly attractive option for its computational efficiency [13, 14]. The PBE is rewritten in terms of moments and one solves for just the first few moments which are usually sufficient for most practical applications [37]. Development of MOM for the fragmentation/breakage process is a particularly active field of research (see, e.g., Refs. [7, 15]). In Ref. [7] the hybrid method of moments (HMOM) [6] is extended to model the fragmentation of soot aggregates in laminar flames. HMOM combines the numerical ease of the method of moments with interpolative closure (MOMIC) [37] and the accuracy of the direct quadrature method of moments (DQMOM) [21] with a source term for the smallest particles based on the negative infinity moment. The production of the smallest particles was assumed to be proportional to the mass lost from the large particles. Symmetric fragmentation was assumed where one particle fragments into two identical particles. In this paper we test HMOM, albeit a spherical particle description, for both

51 symmetric fragmentation and erosion distribution functions.

52 Another widely used moment method that has been used to address  
53 breakage is the quadrature method of moments (QMOM) [17–20] where the  
54 PSD is approximated by a weighted summation of Dirac delta functions. The  
55 performance of QMOM for simultaneous aggregation and breakage problems  
56 with different combinations of aggregation and breakage kernels, fragment  
57 distribution functions and initial conditions has been investigated in Ref. [20].  
58 A quadrature approximation with two nodes was found to be sufficiently ac-  
59 curate for most cases except for symmetric fragmentation with a constant  
60 kernel and erosion with a size-dependent kernel. Increasing the number of  
61 nodes did not help in decreasing the error in some cases. However, across all  
62 cases aggregation was dominant. The accuracy of QMOM in treating pure  
63 breakage problems or where breakage is the dominant process has not been  
64 addressed yet. This paper will be a step in this direction.

65 In Ref. [38] a finite-size domain complete set of trial functions method  
66 of moments (FCMOM) is proposed which uses a series of Legendre polyno-  
67 mials to reconstruct the PSD, thus closing the moment equations. However,  
68 because only a finite number of polynomials can be determined, certain val-  
69 ues of the reconstructed PSD can be negative [39]. An alternative method  
70 is the extended quadrature method of moments (EQMOM) where a set of  
71 non-negative continuous kernel density functions such as gamma, beta and  
72 lognormal functions is adopted to approximate the PSD. In terms of the re-  
73 constructed PSD this method can achieve very high accuracy and is able to  
74 handle the shrinkage problem. However, information about the shape of the  
75 PSD is needed *a priori* to select a suitable kernel density function. Both

76 FCMOM and EQMOM are focused on the reconstruction of the PSD while  
77 for most practical applications only the first few moments are needed.

78 Recently, a moment projection method (MPM) [5] was developed to ad-  
79 dress the shrinkage of particles. It directly solves the moment transport  
80 equation and tracks the number of the smallest particles using the algo-  
81 rithm by Blumstein and Wheeler [40]. A similar algorithm for solving the  
82 Gauss-Radau quadrature is given by Golub [41, 42]. In both algorithms the  
83 derivation is given in terms of orthogonal polynomials which is straightfor-  
84 ward and can be easily modified to treat the cases in which zero, one or two  
85 particle mass classes are fixed. The ability of MPM to simulate shrinkage  
86 problems was investigated and the advantages of the method was highlighted.  
87 To be able to model fragmentation accurately one has to be able to model the  
88 number of the smallest particles accurately which are formed under strong  
89 fragmentation. Therefore, fragmentation is a natural extension of MPM.

90 For quadrature-based moment methods a very important consideration  
91 is the realisability of the moment set [43]. Realisability is related to the  
92 existence of an underlying PSD that corresponds to a set of moments. The  
93 moments are linked to each other under complex mathematical relationships.  
94 If the numerical schemes do not preserve these relationships the set of mo-  
95 ments can be unrealisable, i.e., no PSD can be described by such moments  
96 or they lead to unphysical distributions (e.g. negative weights and abscis-  
97 sas). The generation of unrealizable moments usually arises from the spatial  
98 transportation of moments [44]. Even if a suitable closure is established for  
99 the moment transport equation, numerical advection and diffusion schemes  
100 can still lead to unrealizable moment sets. This realisability problem can be

101 avoided by properly designing the numerical schemes. For example, recently  
102 in Ref. [45] a high-order-volume-schemes for quadrature-based moment meth-  
103 ods is introduced to guarantee the realisability of moments. The idea of the  
104 discretization scheme is to construct the moment flux terms through inter-  
105 polation of the quadrature weights rather than the moments at the faces of  
106 the cells. By doing this the realisability problem can be prevented. Another  
107 scheme developed to preserve the realisability of moments can be found in  
108 Ref. [46] where the moments are not transported directly. Instead they use  
109 the canonical moments which are easy to control and guarantee the moment  
110 vector to stay in the moment space by transporting them separately. In light  
111 of realisability, here we restrict our attention to the moment closure method.  
112 The aim is to investigate the MPM error in isolation. Therefore we are simu-  
113 lating a spatially homogenous PBE with no moment advection and diffusion  
114 terms. The moments always remain realizable during the whole simulation  
115 time span. While for the application of MPM to spatially inhomogeneous  
116 systems, moments realizability can be guaranteed by adopting the realizable  
117 finite-volume methods.

118 In this work, different types of fragmentation kernels, fragment distribu-  
119 tion functions and initial conditions are imposed and the results are compared  
120 with QMOM, HMOM and a high-precision stochastic solution. Both QMOM  
121 and HMOM have the advantages of mathematical simplicity, numerical ro-  
122 bustness and ease of implementation. The stochastic solution was obtained  
123 with 131,072 stochastic particles in a single run and is used as “exact” so-  
124 lution in this work. The paper is organized as follows. Section 2 presents  
125 the moment of methods for solving the PBE as well as the mathematical for-

126 mulation and numerical algorithm of MPM. In Section 3 the performance of  
127 MPM is tested for different test cases and in Section 4 principal conclusions  
128 are summarised.

## 129 **2. Moment methods for population balance equations**

### 130 *2.1. Population balance equation*

131 A spatially homogeneous population of particles with a discrete-mass dis-  
132 tribution is considered in this work. The smallest particles have mass  $m_1$  and  
133 particles in the mass class  $i$  have mass  $m_i = im_1$ . The PBE governing the  
134 evolution of the distribution can be written as:

$$\frac{dN(i, t)}{dt} = R(i, t) + W(i, t) + S(i, t) + G(i, t) + F(i, t), \quad i = 1, 2, \dots, \infty, \quad (1)$$

135 where  $N(i, t)$  is the number of particles in the mass class  $i$  at time  $t$  which  
136 we will refer to as  $N_i$  from hereon. This is known as a particle number  
137 representation of the PSD.  $R$ ,  $W$ ,  $S$ ,  $G$  and  $F$  are the inception, growth,  
138 shrinkage, coagulation and fragmentation terms, respectively. The specific  
139 functional forms used in this work are as follows:

$$R(i = 1, t) = I_{m_1}, \quad (2)$$

$$W(i, t) = K_G(i - \delta)N_{i-\delta} - K_G(i)N_i, \quad (3)$$

$$S(i, t) = K_{Sk}(i + \delta)N_{i+\delta} - K_{Sk}(i)N_i, \quad (4)$$

$$G(i, t) = \frac{1}{2} \sum_{j=1}^i K_{Cg}(j, i - j)N_jN_{i-j} - \sum_{j=1}^{\infty} K_{Cg}(i, j)N_iN_j, \quad (5)$$

$$F(i, t) = \sum_{j=i}^{\infty} K_{Fg}(j)P(i|j)N_j - K_{Fg}(i)N_i, \quad (6)$$

140 where  $I_{m_1}$  is the inception kernel which describes the rate of formation of the  
 141 smallest particles.  $K_G$  and  $K_{Sk}$  are the growth and shrinkage kernels, respec-  
 142 tively, where  $\delta$  refers to the mass change in a single growth or shrinkage event  
 143 which can be different.  $K_{Cg}$  is the coagulation kernel which describes the rate  
 144 at which particles collide and stick together. Lastly,  $K_{Fg}$  is the fragmenta-  
 145 tion kernel which describes the frequency with which particles fragment and  
 146  $P(i|j)$  is the fragment distribution function which represents the number of  
 147 particles of mass class  $i$  formed by the fragmentation of particles of mass  
 148 class  $j$ .

149 The choice of fragmentation kernel and fragment distribution function  
 150 are important because for certain combinations, “shattering” may occur [47,  
 151 48]. In a process analogous to gelation (but in the opposite sense), a finite  
 152 fraction of the mass shatters into an infinite number of particles of zero mass  
 153 and for this reason mass is not conserved [49]. This usually occurs when  
 154 the fragmentation rate increases as the particles become smaller. Note that  
 155 self-similar solutions where the PSD does not vary with time are of special  
 156 interest as the PSD is independent of initial conditions and most experimental



157 systems evolve to the point where this behaviour is reached [50]. It is found  
 158 in Ref. [51] that a self-similar PSD is achieved when the fragmentation kernel  
 159 is of the power type and the fragment distribution function depends on the  
 160 parent-daughter particle mass ratio.

161 Many different functional forms of the fragment distribution function have  
 162 been proposed, however some physical constraints must be fulfilled [51, 52]:

$$P(i|j) = 0, \quad \text{for } i > j, \quad (7)$$

$$\sum_{i=1}^j iP(i|j) = j. \quad (8)$$

163 The first equation states that fragmentation can only lead to the formation  
 164 of particles of mass class  $i$  smaller than the parent particle mass class  $j$ ,  
 165 while the second equation is the conservation of mass where the total mass  
 166 class of particles resulting from the breakup of a particle of mass class  $j$   
 167 must be equal to  $j$ . In this work, we only consider binary fragmentation and  
 168 the fragment distribution functions are reported in Table 1; a discussion of  
 169 multiple fragmentation can be found in Ref. [51]. Symmetric fragmentation  
 170 leads to the formation of two equal mass fragments, whereas in the case of  
 171 erosion one fragment is of the smallest mass class  $i = 1$  while the other is of  
 172 the mass class  $i = j - 1$ .

## 173 2.2. Moment equations

174 As mentioned earlier, an efficient approach for solving the PBE is MOM  
 175 where the PBE is transformed into a set of moment equations and integral  
 176 quantities such as the total particle number and mass are computed. This is  
 177 achieved by applying the definition, moment of order  $k$  of the PSD

**Table 1:** *Fragmentation distribution functions.*

Mechanism	$P(i j)$
Symmetric fragmentation	$\begin{cases} 2 & \text{if } i = j/2 \\ 0 & \text{otherwise} \end{cases}$
Erosion	$\begin{cases} 1 & \text{if } i = 1 \\ 1 & \text{if } i = j - 1 \\ 0 & \text{otherwise} \end{cases}$

$$M_k = \sum_{i=1}^{\infty} i^k N_i, \quad k = 0, 1, 2, \dots, \quad (9)$$

<sup>178</sup> to Eq. (1), leading to

$$\frac{dM_k}{dt} = R_k(M) + G_k(M) + W_k(M) + S_k(M, N_1) + F_k(M, N_1), \quad (10)$$

<sup>179</sup> where

$$R_k(M) = m_1^k I_{m_1}, \quad (11)$$

$$G_k(M) = \frac{1}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{i-1} i^k K_{\text{Cg}}(j, i-j) N_j N_{i-j} - \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} i^k K_{\text{Cg}}(i, j) N_i N_j, \quad (12)$$

$$W_k(M) = \sum_{i=1}^{\infty} K_{\text{G}}(i-\delta) i^k N_{i-\delta} - \sum_{i=1}^{\infty} K_{\text{G}}(i) i^k N_i, \quad (13)$$

$$S_k(M, N_1) = \sum_{i=1}^{\infty} K_{\text{Sk}}(i+\delta) i^k N_{i+\delta} - \sum_{i=1}^{\infty} K_{\text{Sk}}(i) i^k N_i, \quad (14)$$

$$F_k(M, N_1) = \sum_{j=1}^{\infty} \sum_{i=1}^j K_{\text{Fg}}(j) i^k P(i|j) N_j - \sum_{i=1}^{\infty} K_{\text{Fg}}(i) i^k N_i. \quad (15)$$

180 Evaluation of the moment source terms depends on the kernel function  $K$ .  
 181 It is assumed that when the smallest particles shrink they are removed from  
 182 the system, while for the fragmentation process the smallest particles are  
 183 unbreakable. Depending on the specific kernels used the shrinkage and frag-  
 184 mentation source terms  $S_k$  and  $F_k$  can depend on the number of the smallest  
 185 particles  $N_1$ . These will be specified later. Where realistic kernels are used,  
 186 fractional- or even negative-order moments are encountered [14]. Therefore,  
 187 the mathematical difficulty of MOM lies in obtaining closure for these mo-  
 188 ment source terms using a finite set of moments. This requires either *a priori*  
 189 assumptions about the shape of the PSD or a suitable closure scheme. One  
 190 of the more widely used closure methods is MOMIC [37] where closure is  
 191 accomplished by Lagrange polynomial interpolation of the logarithm of the  
 192 whole-order moments whose values are available at each integration step of  
 193 Eq. (10). By separating interpolation for positive- and negative-order mo-

194 ments, MOMIC shows very high accuracy in the treatment of mono-modal  
 195 PSDs undergoing growth and coagulation and satisfactory accuracy for bi-  
 196 modal PSDs formed under persistent nucleation [6]. However, MOMIC can-  
 197 not handle shrinkage as it does not track  $N_1$ . Likewise, it cannot rigorously  
 198 treat fragmentation especially erosion where a large number of particles ac-  
 199 cumulate in the smallest particle mass class.

### 200 *2.3. Moment projection method*

201 The mathematical formulation and numerical algorithm of MPM have  
 202 already been presented in Ref. [5], however, pertinent details are repeated  
 203 here for the reader’s convenience. In MPM, we approximate the true PSD  
 204 by assuming that all particles are distributed into a finite number of particle  
 205 mass classes. The  $k$ -th order moment of the approximated PSD can then be  
 206 expressed as:

$$\widetilde{M}_k = \alpha_1^k \widetilde{N}_{\alpha_1} + \sum_{j=2}^{N_p} \alpha_j^k \widetilde{N}_{\alpha_j}, \quad k = 0, \dots, 2N_p - 2, \quad (16)$$

207 where  $\alpha_j$  is the particle mass,  $\widetilde{N}_{\alpha_j}$  is the number of particles of the mass  
 208  $\alpha_j$ , and  $N_p$  is the number of particle masses used to represent the PSD. The  
 209 symbol “ $\sim$ ” is used to indicate approximations of the corresponding quantity  
 210 from the true PSD.  $\alpha_j$  and  $\widetilde{N}_{\alpha_j}$  are chosen such that the empirical moments  
 211 are equal to the moments from the true PSD:

$$\widetilde{M}_k = M_k. \quad (17)$$

212 Applying Eq. (17) to Eq. (10), we obtain:

$$\frac{d\widetilde{M}_k}{dt} = R_k(\widetilde{M}) + G_k(\widetilde{M}) + W_k(\widetilde{M}) + S_k(\widetilde{M}, N_1) + F_k(\widetilde{M}, N_1). \quad (18)$$

213 To evaluate the boundary flux term  $N_1$  present in the shrinkage and frag-  
 214 mentation terms, we fix the first particle mass to be equal to the smallest  
 215 particle mass of the true PSD:  $\alpha_1 = m_1$ . Therefore,  $\widetilde{N}_{\alpha_1}$  is an approximation  
 216 of the number of the smallest particle which allows us to express Eq. (18) as:

$$\frac{d\widetilde{M}_k}{dt} = R_k(\widetilde{M}) + G_k(\widetilde{M}) + W_k(\widetilde{M}) + S_k(\widetilde{M}, \widetilde{N}_{\alpha_1}) + F_k(\widetilde{M}, \widetilde{N}_{\alpha_1}). \quad (19)$$

217 As can be seen from Eq. (19),  $\widetilde{M}_k$  is directly evaluated from the moment  
 218 transport equation which allows us to take advantage of MOMIC when real-  
 219 istic kernels are used. However, this introduces an interpolation error. The  
 220 aim here is to investigate the MPM error in isolation, therefore constant  
 221 kernels are adopted:

$$R_k(\widetilde{M}) = m_1^k I_{m_1}, \quad k = 0, \dots, 2N_p - 2, \quad (20)$$

$$G_k(\widetilde{M}) = \begin{cases} -\frac{1}{2} K_{\text{Cg}} \widetilde{M}_0^2, & k = 0, \\ 0, & k = 1, \\ \frac{1}{2} K_{\text{Cg}} \sum_{r=1}^{k-1} \binom{k}{r} \widetilde{M}_r \widetilde{M}_{k-r}, & k = 2, \dots, 2N_p - 2, \end{cases} \quad (21)$$

$$W_k(\widetilde{M}) = \begin{cases} 0, & k = 0, \\ K_G \sum_{r=1}^k \binom{k}{r} \delta^r \widetilde{M}_{k-r}, & k = 1, \dots, 2N_p - 2, \end{cases} \quad (22)$$

$$S_k(\widetilde{M}, \widetilde{N}_{\alpha_1}) = \begin{cases} -K_{\text{Sk}}\widetilde{N}_{\alpha_1}, & k = 0, \\ K_{\text{Sk}} \sum_{r=1}^k \binom{k}{r} (-\delta)^r \widetilde{M}_{k-r}, & k = 2, \dots, 2N_p - 2. \end{cases} \quad (23)$$

222 The fragmentation source term depends on the fragment distribution  
 223 function. For symmetric fragmentation it is:

$$F_k(\widetilde{M}, \widetilde{N}_{\alpha_1}) = \begin{cases} K_{\text{Fg}}(\widetilde{M}_0 - \widetilde{N}_{\alpha_1}), & k = 0, \\ 0, & k = 1, \\ K_{\text{Fg}}(2^{1-k} - 1)(\widetilde{M}_k - \alpha_1^k \widetilde{N}_{\alpha_1}), & k = 2, \dots, 2N_p - 2, \end{cases} \quad (24)$$

224 and for erosion:

$$F_k(\widetilde{M}, \widetilde{N}_{\alpha_1}) = \begin{cases} K_{\text{Fg}}(\widetilde{M}_0 - \widetilde{N}_{\alpha_1}), & k = 0 \\ 0, & k = 1, \\ K_{\text{Fg}}\alpha_1^k \widetilde{M}_0 + K_{\text{Fg}} \sum_{r=1}^k \binom{k}{r} (-\alpha_1)^r \widetilde{M}_{k-r}, & k = 2, \dots, 2N_p - 2. \end{cases} \quad (25)$$

225 In Ref. [30] a fragmentation kernel with a linear dependence on particle  
 226 mass is used to study the wet granulation of particles. Since the fragmen-  
 227 tation moment source term can be evaluated based on the whole-moments,  
 228 we also investigate the same fragmentation kernel which for symmetric frag-  
 229 mentation is:

$$F_k(\widetilde{M}, \widetilde{N}_{\alpha_1}) = \begin{cases} K_{\text{Fg}}(\widetilde{M}_1 - \alpha_1 \widetilde{N}_{\alpha_1}), & k = 0, \\ 0, & k = 1, \\ K_{\text{Fg}}(2^{1-k} - 1)(\widetilde{M}_{k+1} - \alpha_1^{k+1} \widetilde{N}_{\alpha_1}), & k = 2, \dots, 2N_p - 2, \end{cases} \quad (26)$$

230 and for erosion:

$$F_k(\widetilde{M}, \widetilde{N}_{\alpha_1}) = \begin{cases} K_{\text{Fg}}(\widetilde{M}_1 - \alpha_1 \widetilde{N}_{\alpha_1}), & k = 0, \\ 0, & k = 1, \\ K_{\text{Fg}}\alpha_1^k \widetilde{M}_1 + K_{\text{Fg}} \sum_{r=1}^k \binom{k}{r} (-\alpha_1)^r \widetilde{M}_{k-r+1}, & k = 2, \dots, 2N_p - 2. \end{cases} \quad (27)$$

231 The challenge now is determining  $\alpha_j$  and  $\widetilde{N}_{\alpha_j}$  such that Eq. (17) is true  
 232 while fulfilling the requirement that  $\widetilde{N}_{\alpha_1} \cong N_1$  to close the moment source  
 233 terms due to shrinkage and fragmentation. This can be achieved using the  
 234 Blumstein and Wheeler algorithm [40] which can be found in Appendix 2.  
 235 The numerical procedure of MPM is summarized in Algorithm 1.

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**Algorithm 1:** Moment projection method algorithm.

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**Input:** Moments of the PSD  $M_k(t_0)$  for  $k = 0, \dots, 2N_p - 2$  or the PSD itself

$N(i, t_0)$  for  $i = 1, \dots, \infty$  at initial time  $t_0$ ; final time  $t_f$ .

**Output:** Empirical moments of the PSD  $\widetilde{M}_k(t_f)$  for  $k = 0, \dots, 2N_p - 2$  at final time  $t_f$  where  $N_p$  is the number of particle masses used to approximate the PSD.

Calculate the moments of the true PSD using Eq. (9):

$$M_k(t_0) = \sum_{i=1}^{\infty} i^k N(i, t_0), \quad k = 0, \dots, 2N_p - 2.$$

For  $\widetilde{M}_k = M_k$ , solve Eq. (16) for  $\widetilde{N}_{\alpha_1}$  ( $\alpha_1$  is fixed) and  $\alpha_j$  and  $\widetilde{N}_{\alpha_j}$  ( $j = 2, \dots, N_p$ ) using Algorithm 2:

$$\widetilde{M}_k(t_0) = \alpha_1^k \widetilde{N}_{\alpha_1}(t_0) + \sum_{j=2}^{N_p} \alpha_j^k \widetilde{N}_{\alpha_j}(t_0), \quad k = 0, \dots, 2N_p - 2.$$

$t \leftarrow t_0, \widetilde{M}_k(t) \leftarrow \widetilde{M}_k(t_0);$

**while**  $t < t_f$  **do**

236

Integrate Eq. (19) over the time interval  $[t_i, t_i + h]$  using a fourth-order Runge-Kutta method:

$$\frac{d\widetilde{M}_k}{dt} = R_k(\widetilde{M}) + G_k(\widetilde{M}) + W_k(\widetilde{M}) + S_k(\widetilde{M}, \widetilde{N}_{\alpha_1}) + F_k(\widetilde{M}, \widetilde{N}_{\alpha_1})$$

with initial condition:

$$\begin{pmatrix} \widetilde{M}_k(t_i) \\ \widetilde{N}_{\alpha_1}(t_i) \end{pmatrix} = \begin{pmatrix} \widetilde{M}_{k,i} \\ \widetilde{N}_{\alpha_1,i} \end{pmatrix},$$

where  $R_k(\widetilde{M})$ ,  $G_k(\widetilde{M})$ ,  $W_k(\widetilde{M})$  and  $S_k(\widetilde{M}, \widetilde{N}_{\alpha_1})$  are given by Eqs. (20), (21), (22) and (23), respectively. The form of  $F_k(\widetilde{M}, \widetilde{N}_{\alpha_1})$  depends on the fragmentation kernel and fragment distribution function as given by Eqs. (24–27).

Use Blumstein algorithm to update  $\alpha_j$  and  $\widetilde{N}_{\alpha_j}$ , and assign solution at

$t_{i+1} = t_i + h:$

$$\begin{pmatrix} \widetilde{M}_{k,i+1} \\ \widetilde{N}_{\alpha_1,i+1} \end{pmatrix} \leftarrow \begin{pmatrix} \widetilde{M}_k(t_i + h) \\ \widetilde{N}_{\alpha_1}(t_i + h) \end{pmatrix}.$$

$i \leftarrow i + 1;$

---



### 237 **3. Numerical results**

238 As the focus of this paper is to test MPM for the process of fragmentation,  
239 we devise a number of test cases which can be classified into the following  
240 three categories: (1) pure fragmentation, (2) simultaneous coagulation and  
241 fragmentation, and (3) all particle processes combined (inception, growth,  
242 coagulation, shrinkage and fragmentation). It is assumed that the smallest  
243 particles are unbreakable, i.e.,  $K_{\text{Fg}}(i = 1) = 0$ . Log-normal, unimodal and  
244 parabolic PSDs are supplied as the initial condition.

245 Numerical results are compared to those from HMOM, QMOM and a  
246 high-precision stochastic solution calculated using the direct simulation al-  
247 gorithm (DSA). HMOM was originally developed for bivariate PBEs [6, 7].  
248 We modify this method so that it is applicable to monovariate PBEs. Details  
249 on the modifications made, with a focus on the fragmentation process, can  
250 be found in Appendix B.

#### 251 *3.1. Pure fragmentation*

252 The fragmentation kernels, fragment distribution functions and initial  
253 conditions used to test pure fragmentation are reported in Table 2.

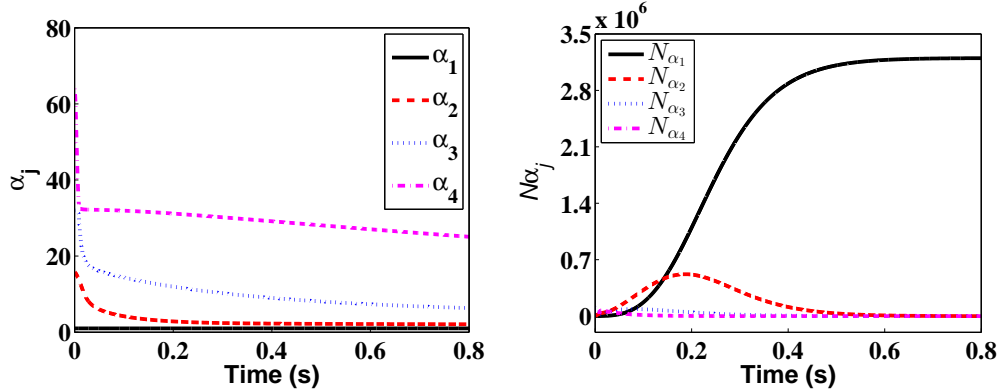
254 For Case 1 particles undergo symmetric fragmentation with a constant  
255 kernel; a log-normal distribution is supplied as the initial condition. The  
256 moment transport equation with the fragmentation moment source term in  
257 Eq. (24) is solved. The particle masses  $\alpha_j$  and the corresponding number  
258 of particles  $\tilde{N}_{\alpha_j}$  describing the evolution of the moments of the PSD are  
259 computed using MPM and are shown in Fig. 1. Four particle masses are  
260 used to approximate the PSD.  $\alpha_j$  ( $j = 2, 3, 4$ ) decrease as particles fragment

**Table 2:** Cases used for the comparison of pure fragmentation.

Case	$K_{\text{Fg}}(i)$	$P(i j)$	$N_i(t = 0)$
1	$\left\{ \begin{array}{l} 0 \quad i = 1 \\ 20 \quad i > 1 \end{array} \right.$	Symmetric fragmentation	$N_i = 10^5 \exp(-(\log(2^{i-1}) - \log(32))^2/0.05)$ , $i = 1, \dots, 10$
2	$\left\{ \begin{array}{l} 0 \quad i = 1 \\ 2i \quad i > 1 \end{array} \right.$	Erosion	$N_i = 100, i = 30$
3	$\left\{ \begin{array}{l} 0 \quad i = 1 \\ 0.2i \quad i > 1 \end{array} \right.$	Symmetric fragmentation	$N_i = 10^5 \exp(-(\log(2^{i-1}) - \log(16))^2/0.05)$ , $i = 1, \dots, 10$
4	$\left\{ \begin{array}{l} 0 \quad i = 1 \\ 0.2i \quad i > 1 \end{array} \right.$	Symmetric fragmentation	$N_i = 10000, i = 256$
5	$\left\{ \begin{array}{l} 0 \quad i = 1 \\ 2 \quad i > 1 \end{array} \right.$	Erosion	$N_i = 300i - 10i^2, i = 1, \dots, 30$
6	$\left\{ \begin{array}{l} 0 \quad i = 1 \\ 2 \quad i > 1 \end{array} \right.$	Erosion	$N_i = 100 \exp(-(\log(i) - \log(25))^2/0.05)$ , $i = 1, \dots, 100$
7	$\left\{ \begin{array}{l} 0 \quad i = 1 \\ 2i \quad i > 1 \end{array} \right.$	Erosion	$N_i = 100 \exp(-(\log(i) - \log(25))^2/0.05)$ , $i = 1, \dots, 100$

261 to form increasingly smaller particles. The number of particles of the largest  
262 mass  $\tilde{N}_{\alpha_4}$  decreases leading to an initial increase in  $\tilde{N}_{\alpha_2}$  and  $\tilde{N}_{\alpha_3}$  before also  
263 decreasing.  $\tilde{N}_{\alpha_1}$  increases and shows an asymptote at around  $N = 3.0 \times 10^6$   
264 as particles of the smallest mass  $m_1$  are formed which are assumed to not be  
265 able to fragment further.

266 To assess the accuracy of the moments calculated using MPM the follow-  
267 ing relative error metric is used:

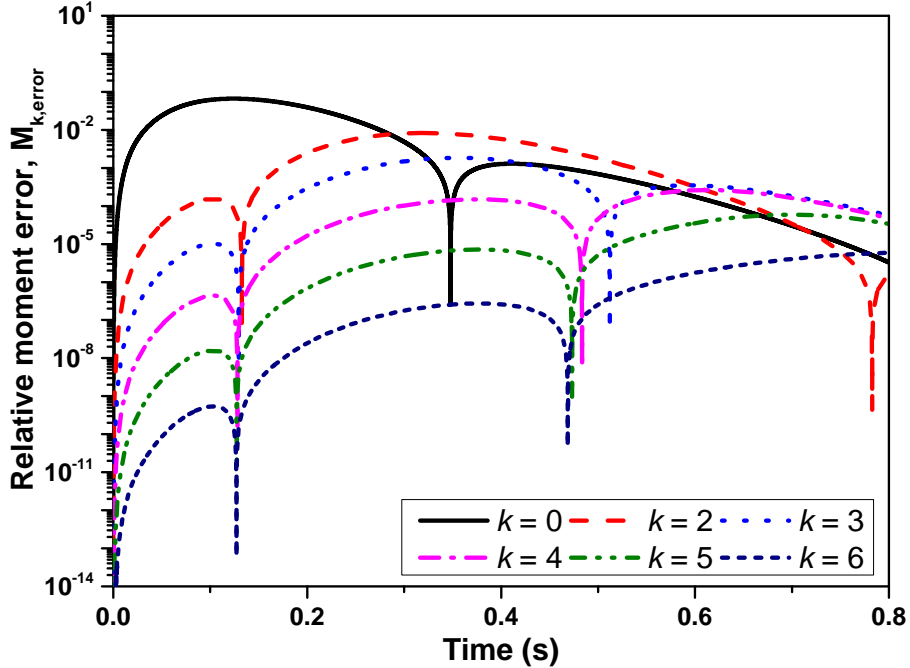


**Figure 1:** Evolution of the particle mass  $\alpha_j$  (left panel) and the corresponding number of particles  $N_{\alpha_j}$  (right panel) obtained using MPM for case 1.

$$M_{k,\text{error}} = \frac{|\widetilde{M}_k - M_k|}{M_k}, \quad (28)$$

268 where  $M_k$  is the  $k$ -th order moment from a high-precision stochastic solution.  
 269 Figure 2 shows the relative moment errors computed using MPM with  $N_p = 4$   
 270 for case 1.  $M_{k,\text{error}}$  shows cusp points when the function  $(\widetilde{M}_k - M_k)$  changes  
 271 sign which was also observed in Ref. [20] for QMOM. In general, MPM shows  
 272 very high accuracy. Although the relative errors in the higher-order moments  
 273 ( $k = 5, 6$ ) show an overall increase, the errors at  $t = 0.8$  s is at most  $10^{-4}$ .  
 274 By contrast, the relative errors in the lower-order moments ( $k = 0, 2$ ) show  
 275 an overall decrease. Note that as mass is conserved in MPM the errors in  
 276 the first-order moment (total particle mass) is 0.

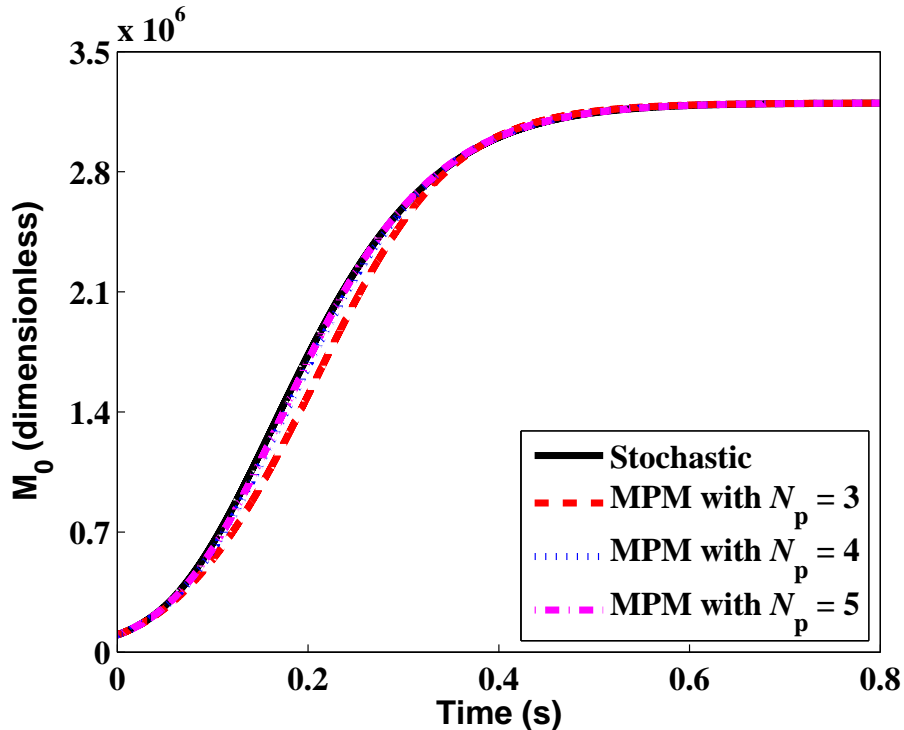
277 To investigate the sensitivity of the results to the number of particle  
 278 masses,  $N_p$ , moments are computed using MPM with  $N_p = 3, 4$  and  $5$  and  
 279 compared with the stochastic solution. Figure 3 shows that for case 1 at  
 280 least four particle masses (dotted line) are required for there to be no obvious



**Figure 2:** Error in the  $k$ -th order moment obtained using MPM relative to a high-precision stochastic solution for case 1.

281 discrepancy in  $\widetilde{M}_0$ . Interestingly,  $\widetilde{M}_0$  at longer residence times displays little  
 282 sensitivity to  $N_p$ . The time-averaged ( $t = 0$  to  $0.8$  s) relative moment errors,  
 283  $M_{k,error}$ , as a function of  $N_p$  and  $k$  for case 1 are listed in Table 3. As expected,  
 284 higher accuracy is generally observed when more particle masses are used:  
 285 there is about an order-of-magnitude decrease in the errors in the lower order  
 286 moments ( $k = 0, 2, 3$ ) when  $N_p$  is increased from 3 to 5. However, this is  
 287 not the case for the higher order moments ( $k = 4, 5, 6$ ) where there is in fact  
 288 an increase in errors when  $N_p$  is increased from 4 to 5.

289 For Case 2 particles undergo erosion where the parent particle mass class  
 290 is reduced by one and a particle of the smallest mass class is formed. The

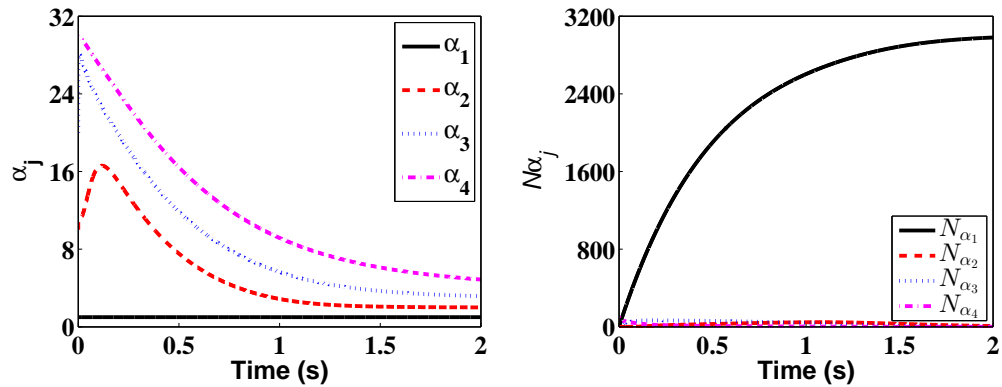


**Figure 3:** Sensitivity of the zeroth moment  $M_0$  to the number of particle masses  $N_p$  obtained using MPM for case 1. The stochastic solution (continuous line) is shown as a point of reference.

291 rate is controlled by a mass-dependent kernel and a unimodal distribution is  
 292 supplied as the initial condition. The moment transport equation with the  
 293 fragmentation moment source term in Eq. (27) is solved. The time evolution  
 294 of  $\alpha_j$  and  $\tilde{N}_{\alpha_j}$  obtained using MPM is shown in Fig. 4. At  $t = 0$ , the third  
 295 and fourth particle masses are positioned on either side of the particles at  
 296 mass class  $i = 30$ . As these particles reduce in mass,  $\alpha_j$  ( $j = 2, 3, 4$ ) all move  
 297 towards the position of the new parent particle class to better represent these  
 298 particles. This is reflected as an increase in  $\alpha_2$  (and  $\alpha_3$ ) and a decrease in  
 299  $\alpha_4$ . The evolution of  $\tilde{N}_{\alpha_j}$  is similar to that of case 1.

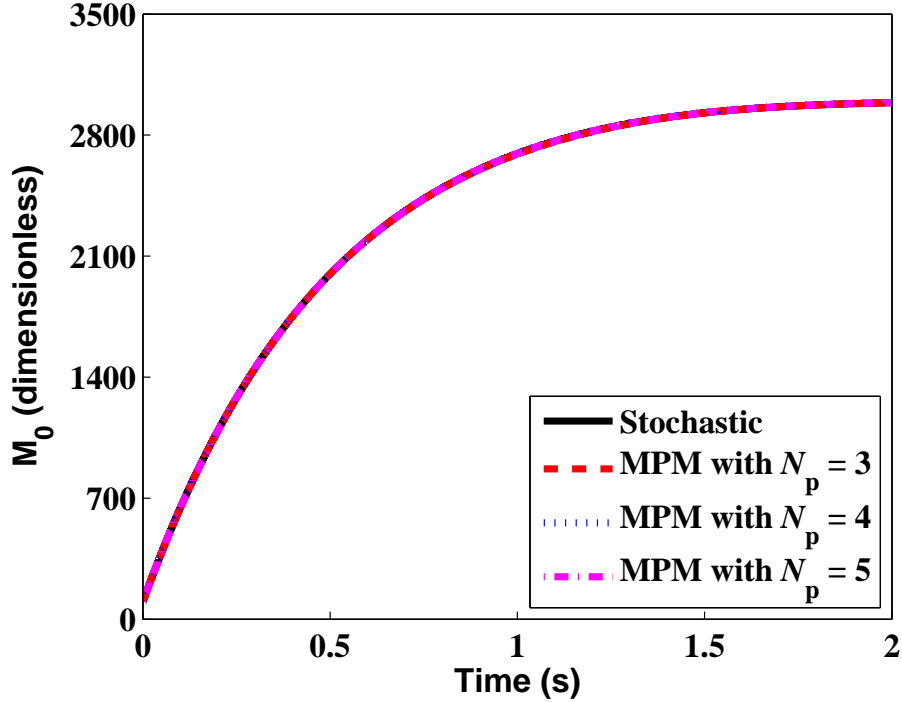
**Table 3:** Average error in the  $k$ -th order moment obtained using MPM relative to a high-precision stochastic solution for different particle masses  $N_p$  for case 1.

$k$	$N_p = 3$	$N_p = 4$	$N_p = 5$
0	$3.9 \times 10^{-2}$	$1.3 \times 10^{-2}$	$8.2 \times 10^{-3}$
1	0	0	0
2	$8.8 \times 10^{-3}$	$2.3 \times 10^{-3}$	$9.7 \times 10^{-4}$
3	$2.3 \times 10^{-3}$	$5.2 \times 10^{-4}$	$2.1 \times 10^{-4}$
4	$4.0 \times 10^{-4}$	$9.6 \times 10^{-5}$	$2.3 \times 10^{-4}$
5	-	$1.6 \times 10^{-5}$	$2.8 \times 10^{-4}$
6	-	$1.2 \times 10^{-6}$	$3.1 \times 10^{-4}$
7	-	-	$3.1 \times 10^{-4}$
8	-	-	$3.2 \times 10^{-4}$



**Figure 4:** Evolution of the particle mass  $\alpha_j$  (left panel) and the corresponding number of particles  $N_{\alpha_j}$  (right panel) computed using MPM for case 2.

300 Figure 5 shows the sensitivity of  $M_0$  to the number of particle masses  
 301 computed using MPM for case 2. It can be seen that there is no discernable



**Figure 5:** *Sensitivity of the zeroth moment  $M_0$  to the number of particle masses  $N_p$  obtained using MPM for case 2. The stochastic solution (continuous line) is shown as a point of reference.*

302 difference between MPM and the stochastic method across all particle masses.  
 303 This is due to the mass-dependent kernel used where the only source of error  
 304 in the fragmentation moment source term  $F_k(\tilde{M}, \tilde{N}_{\alpha_1})$  is in  $\tilde{N}_{\alpha_1}$  (see Eqs. (26)  
 305 and (27) for  $k = 0$ ) as opposed to both  $\tilde{M}_0$  and  $\tilde{N}_{\alpha_1}$  for mass-independent  
 306 kernels (see Eqs. (24) and (25) for  $k = 0$ ) such as in case 1. The time-  
 307 averaged relative errors ( $t = 0$  to 2 s) are listed in Table 4. Overall, the  
 308 errors are lower than in case 1 but the observations that can be made are  
 309 similar. Note that each increment in the number of particle masses requires  
 310 the solution of two extra moments (See Eq. (16)). Smaller tolerances have to

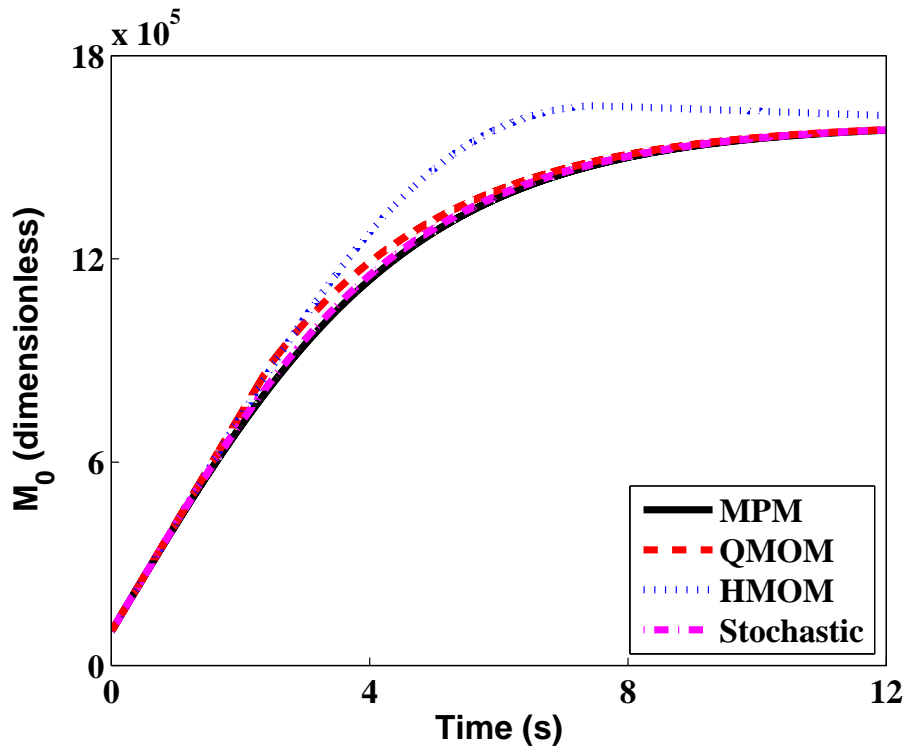
**Table 4:** Average error in the  $k$ -th order moment obtained using MPM relative to a high-precision stochastic solution for different particle masses  $N_p$  for case 2.

k	$N_p = 3$	$N_p = 4$	$N_p = 5$
0	$2.7 \times 10^{-4}$	$1.1 \times 10^{-4}$	$1.5 \times 10^{-5}$
1	0	0	0
2	$3.6 \times 10^{-6}$	$8.4 \times 10^{-8}$	$5.9 \times 10^{-8}$
3	$1.9 \times 10^{-6}$	$8.3 \times 10^{-8}$	$6.7 \times 10^{-8}$
4	$1.8 \times 10^{-6}$	$5.8 \times 10^{-8}$	$9.3 \times 10^{-8}$
5	-	$5.4 \times 10^{-8}$	$9.6 \times 10^{-8}$
6	-	$5.3 \times 10^{-8}$	$9.4 \times 10^{-8}$
7	-	-	$8.8 \times 10^{-8}$
8	-	-	$8.1 \times 10^{-8}$

311 be used for the time integration of the set of ODEs and increases the stiffness  
312 of the eigenvalue-eigenvector problem solved via the Blumstein and Wheeler  
313 algorithm, thus leading to a higher computational cost. For this reason, four  
314 particle masses will be used in the rest of this paper.

315 Case 3 is similar to case 2 except that a mass-dependent kernel is used.  
316 The moment transport equation with the fragmentation moment source term  
317 in Eq. (26) is solved. We now compare MPM to other moment methods:  
318 HMOM and QMOM with four nodes. Figure 6 shows a comparison of  $M_0$  be-  
319 tween MPM, HMOM and QMOM with the stochastic solution as a reference.  
320 There is an excellent agreement between MPM and the stochastic method  
321 apart from a slight underprediction at intermediate times. Both HMOM  
322 and QMOM overestimate  $M_0$  but the performance by HMOM is worse. It

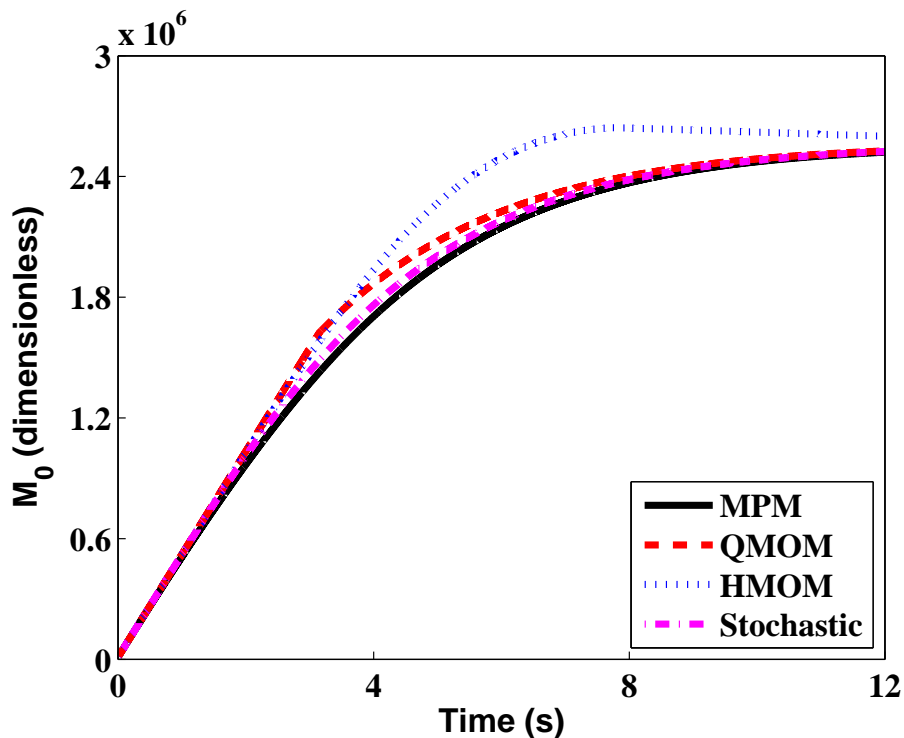




**Figure 6:** Comparison of the zeroth moment  $M_0$  between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic solution for case 3.

323 was initially puzzling but it became clear to us that in HMOM particles are  
 324 represented as either small or large particles which is a coarser assumption  
 325 than the four particles masses or nodes used in MPM and QMOM, respec-  
 326 tively. Second, it is assumed that the rate at which the smallest particles are  
 327 formed is proportional to the overall fragmentation rate [7]. However, there  
 328 exist situations where particles fragment and the smallest particles are not  
 329 formed, for example, in symmetric fragmentation. Although QMOM incurs  
 330 some errors, when particles are small enough, it implicitly tracks the number  
 331 of the smallest particles which keeps its accuracy high. The results for case 4

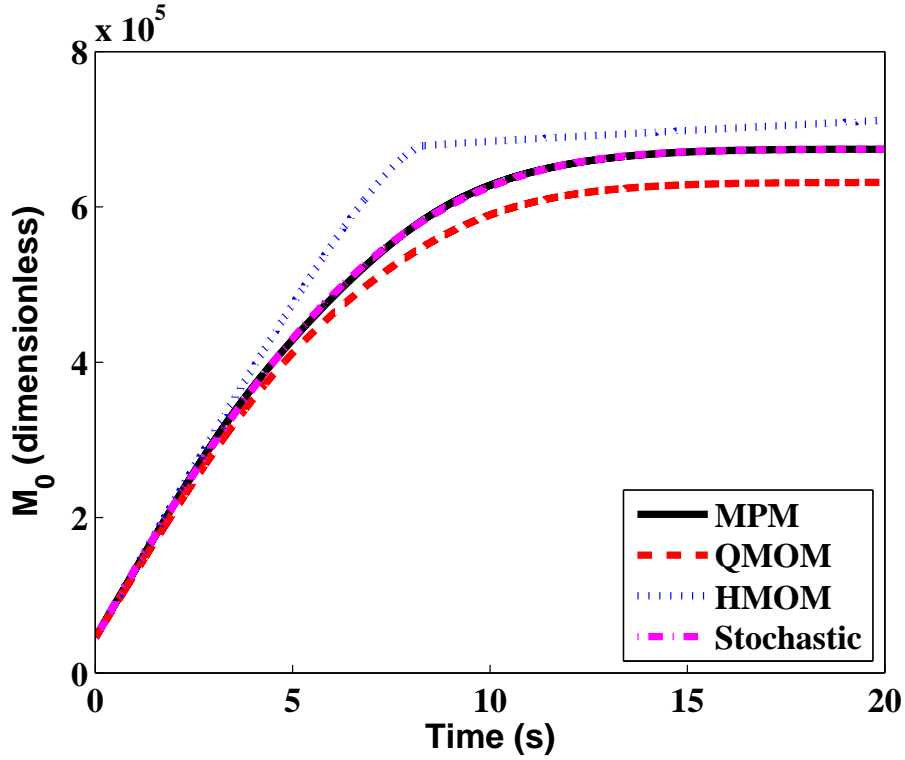
332 where a unimodal distribution is supplied as the initial condition is similar  
 (see Fig. 7).



**Figure 7:** Comparison of the zeroth moment  $M_0$  between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic solution for case 4.

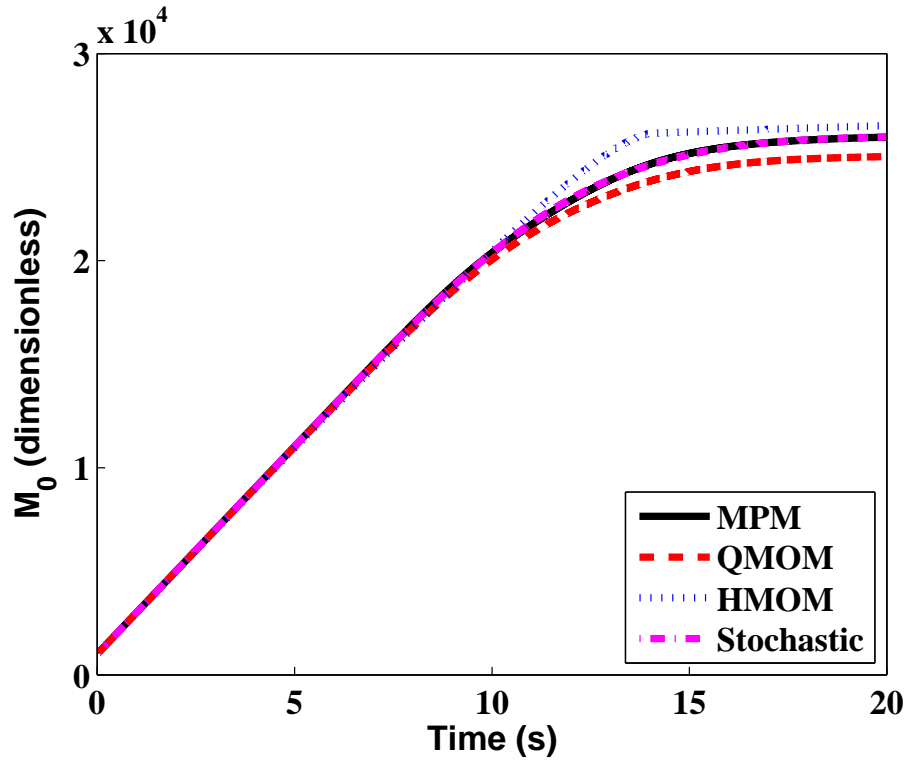
333

334 For case 5, particles undergo erosion with a constant kernel and the mo-  
 335 ment transport equation with the fragmentation source term in Eq. (25) is  
 336 solved. Unlike case 2 where there are only particles at mass class  $i = 30$  at  
 337  $t = 0$  s, the parabolic distribution for this case has particles in the small-  
 338 est mass class. Therefore, the ability to accurately track the number of the  
 339 smallest particles is particularly important. Both HMOM and QMOM are  
 340 not able to even capture the steady-state  $M_0$  at  $t = 20$  s as shown in Fig. 8.



**Figure 8:** Comparison of the zeroth moment  $M_0$  between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic solution for case 5.

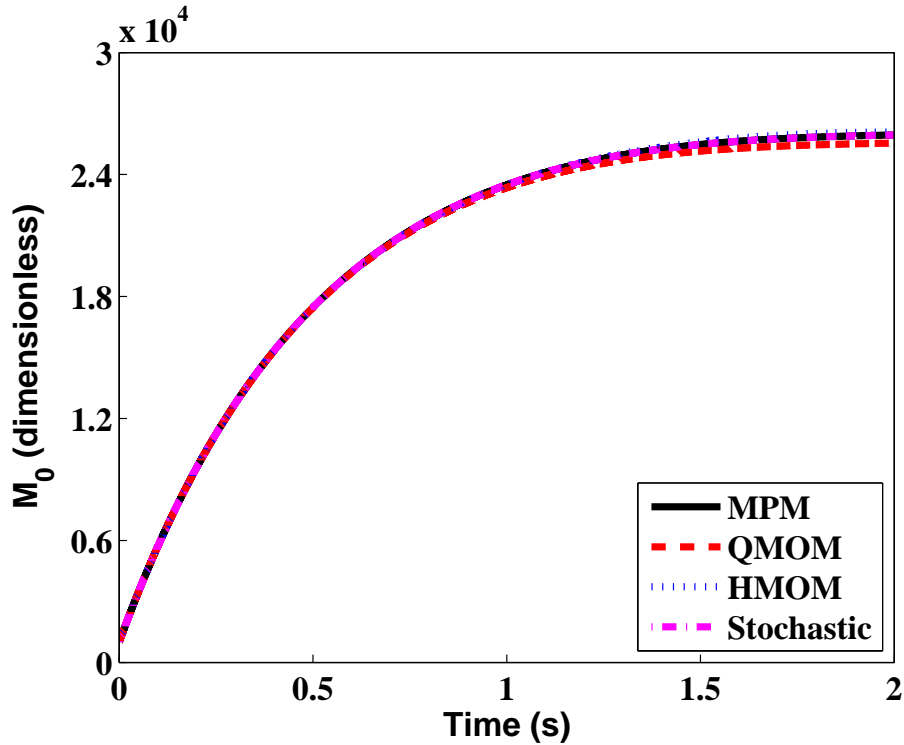
341 For cases 6 and 7, particles undergo erosion and a log-normal distribution  
 342 is supplied as the initial condition. A constant fragmentation kernel is used  
 343 in case 6 while a mass-dependent fragmentation kernel is used in case 7.  
 344  $M_0$  computed using the different methods for cases 6 and 7 are shown in  
 345 Figs. 9 and 10, respectively. The results for case 6 is similar to case 5  
 346 where HMOM overpredicts and QMOM underpredicts  $M_0$ . When a mass-  
 347 dependent fragmentation kernel is used in Case 7, the agreement is much  
 348 improved. As highlighted before, one reason for the improved performance is  
 349 that when the mass-dependent kernel is used, the source term for the zeroth-



**Figure 9:** Comparison of the zeroth moment  $M_0$  between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic solution for case 6.

350 order moment is governed by the total particle mass which is insensitive to  
 351 the number of the smallest particles, thus decreasing the errors in computing  
 352 the moments. In both cases, MPM exhibits the highest accuracy regardless  
 353 of the fragmentation kernel used.

354 Based on the above results, the following observations can be made: MPM  
 355 is the most accurate amongst the different method of moments studied for  
 356 the pure fragmentation process. Across all of these test cases, the agreement  
 357 between  $M_0$  obtained using MPM and the stochastic method is excellent. The  
 358 source term developed in HMOM tends to overestimate the formation of the



**Figure 10:** Comparison of the zeroth moment  $M_0$  between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic solution for case 7.

359 smallest particles. Because QMOM does not explicitly track the number of  
 360 the smallest particles, the performance of QMOM is worse for erosion than  
 361 for symmetric fragmentation.

### 362 3.2. Simultaneous coagulation and fragmentation

363 In this section, the performance of MPM is tested for simultaneous co-  
 364 agulation and fragmentation processes. Depending on the coagulation and  
 365 fragmentation kernels used, the PSD will evolve differently and result in dif-  
 366 ferent total particle numbers at steady state. Four cases are developed to  
 367 investigate the competition between these two processes as shown in Table 5.

The fragmentation kernel is systematically varied while the coagulation ker-

**Table 5:** Cases used for the comparison of simultaneous coagulation and fragmentation.

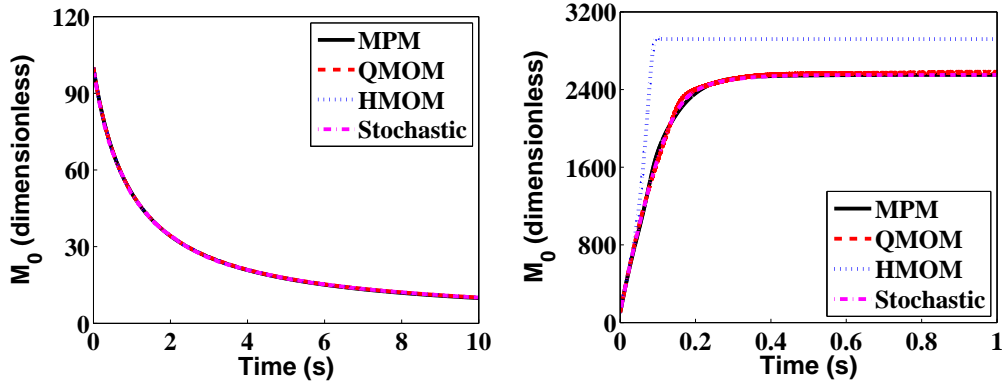
Case	$K_{\text{Fg}}(i)$
8	$\begin{cases} 0 & i = 1 \\ 0.02 & i > 1 \end{cases}$
9	$\begin{cases} 0 & i = 1 \\ 200 & i > 1 \end{cases}$
10	$\begin{cases} 0 & i = 1 \\ 0.02i & i > 1 \end{cases}$
11	$\begin{cases} 0 & i = 1 \\ 200i & i > 1 \end{cases}$

Note:  $K_{\text{Cg}} = 0.02 \text{ s}^{-1}$ ,  $P(i|j) = \text{erosion}$ ,  $N_{30}(t = 0) = 100$ .

368

369 nel is left unchanged. For all of these cases, fragmentation takes the form  
 370 of erosion and the unimodal distribution in case 2 is supplied as the initial  
 371 condition.

372 For case 8, the coagulation and fragmentation kernels are identical.  $M_0$   
 373 computed using the different methods are shown in the left panel of Fig. 11.  
 374 The process is dominated by coagulation as shown by the decrease in  $M_0$ .  
 375 Therefore, very few particles accumulate in the first particle mass class as  
 376 these particles tend to collide with each other to form particles of larger  
 377 mass. Since constant kernels are used, no closure problem is present in the  
 378 coagulation moment equation and all the methods generate almost the same  
 379 results as the stochastic method. Also shown in Fig. 11 (right panel) are the  
 380 corresponding results for case 9 where the fragmentation kernel is four orders-

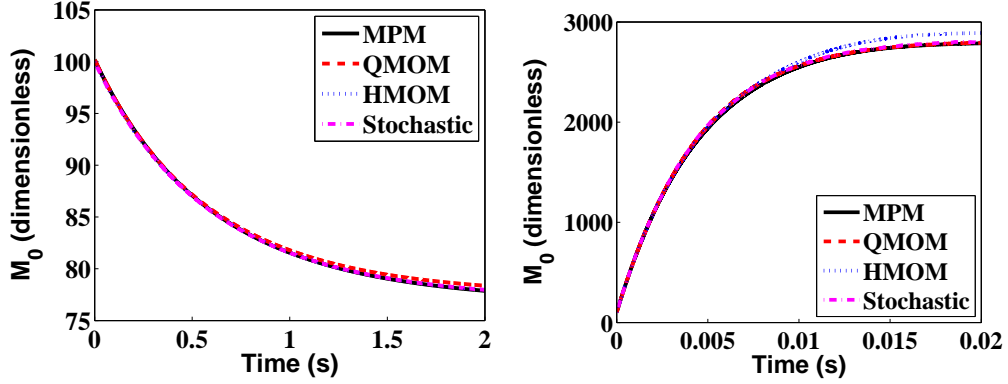


**Figure 11:** Comparison of the zeroth moment  $M_0$  between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic method for case 8 (left panel) and case 9 (right panel).

381 of-magnitude larger than the coagulation kernel. The process is dominated  
 382 by fragmentation and the accumulation of the smallest particles plays an im-  
 383 portant role: HMOM overestimates the formation of the smallest particles,  
 384 thus overestimating  $M_0$ ; MPM shows the highest accuracy while slight dis-  
 385 crepancy is observed between the QMOM and stochastic solutions. Cases 10  
 386 and 11 are similar to cases 8 and 9 except that mass-dependent fragmentation  
 387 kernels are used. Similar conclusions can be drawn from Fig. 12.

### 388 3.3. Combined processes

389 In this section, MPM is tested against QMOM, HMOM and the stochas-  
 390 tic method for the combined processes of inception, growth, coagulation,  
 391 shrinkage and fragmentation. The specifics of the two test cases are shown  
 392 in Table 6. The total particle number and mass of particles computed using  
 393 the different methods for cases 12 and 13 are shown in Figs. 13 and 14, re-  
 394 spectively. It can be seen that MPM exhibits a very high accuracy that was



**Figure 12:** Comparison of the zeroth moment  $M_0$  between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic method for case 10 (left panel) and case 11 (right panel).

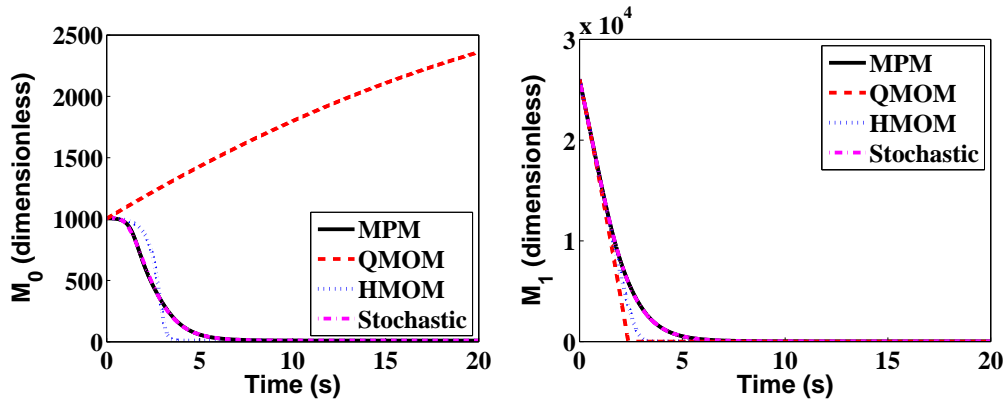
**Table 6:** Cases used for the comparison of combined processes.

Case	$K_{\text{Fg}}(i)$	$N_i(t = 0)$
12	$\begin{cases} 0 & i = 1 \\ 2 \times 10^{-5}i & i > 1 \end{cases}$	$\begin{cases} 100 \exp(-(\log(i) - \log(25))^2/0.05), & i = 1, \dots, 100 \end{cases}$
13	$\begin{cases} 0 & i = 1 \\ 2 \times 10^{-5} & i > 1 \end{cases}$	$N_i = 1000, i = 50$

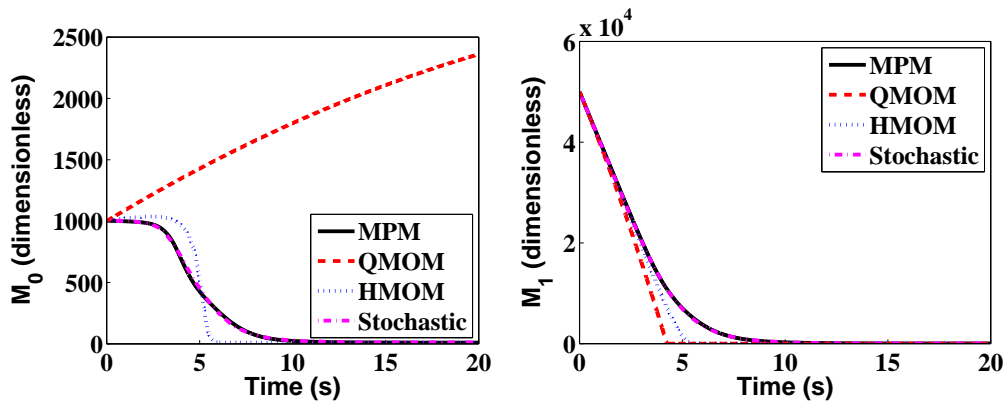
Note:  $I_{m_1} = 100 \text{ s}^{-1}$ ,  $K_G = 20 \text{ s}^{-1}$ ,  $K_{\text{Cg}} = 2 \times 10^{-5} \text{ s}^{-1}$ ,  $K_{\text{Sk}} = 30 \text{ s}^{-1}$  and  $P(i|j) = \text{erosion}$ .

395 also observed for pure fragmentation and simultaneous coagulation and frag-  
396 mentation.  $M_0$  decreases mainly due to the shrinkage of particles—rather  
397 than coagulation—as evidenced by the corresponding decrease in  $M_1$ . The  
398 shrinkage process leads to a zeroth order moment equation containing a term  
399 corresponding to the loss of particles of the smallest size [12, 39]. In order to





**Figure 13:** Comparison of the zeroth order moment  $M_0$  (left panel) and the first order moment  $M_1$  (right panel) between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic method for case 12.



**Figure 14:** Comparison of the zeroth order moment  $M_0$  (left panel) and the first order moment  $M_1$  (right panel) between MPM (four particle masses), QMOM (four nodes), HMOM and the stochastic method for case 13.

400 evaluate this term, the value of the PSD at the smallest internal coordinate is  
 401 required which is not available in QMOM. As expected, Figs. 13 and 14 show  
 402 that QMOM fails to predict the evolution of  $M_0$  and therefore  $M_1$ . Although  
 403 HMOM is able to predict the consumption of particles, it shows a significant

404 discrepancy compared with the stochastic solution.

#### 405 **4. Conclusion**

406 In this paper, the moment projection method (MPM) was extended to  
407 include the fragmentation process. MPM was tested against cases involving  
408 (1) pure fragmentation, (2) simultaneous coagulation and fragmentation, and  
409 (3) combined processes of inception, growth, coagulation, shrinkage and frag-  
410 mentation with different fragmentation kernels, fragment distribution func-  
411 tions and initial conditions. The numerical results were compared against  
412 the hybrid method of moments (HMOM) and the quadrature method of  
413 moments (QMOM) with four nodes and a high-precision stochastic solution  
414 calculated using the direct simulation algorithm (DSA).

415 By fixing the first particle mass  $\alpha_1$  to be equal to the smallest particle  
416 mass  $m_1$ , the evolution of the smallest particles could be tracked in MPM  
417 with a high accuracy. The accuracy was shown to generally improve with the  
418 number of particle masses,  $N_p$ , with  $N_p = 4$  being the best compromise be-  
419 tween accuracy and computational efficiency. In all the test cases considered  
420 in this work, MPM is capable of accurately predicting the time evolution of  
421 the moments while the agreement with HMOM and QMOM tend to be less  
422 good when fragmentation dominates. Future work includes application of  
423 MPM to real particle processes such as soot formation in flames. It remains  
424 to be seen how effective is MPM for more complicated PBEs with additive  
425 kernels and/or free-molecular Brownian kernel.

#### 426 **Acknowledgement**

427 This research is supported by the National Research Foundation, Prime  
428 Minister's Office, Singapore under its CREATE programme.

429 **Nomenclature**

*Upper-case Roman*

- D** Eigenvectors of matrix **P**
  - F* Source term due to fragmentation
  - G* Source term due to coagulation
  - $I_{m_1}$  Inception rate of particles of the smallest mass  $m_1$
  - $K_{Cg}$  Coagulation kernel
  - $K_{Fg}$  Fragmentation kernel
  - $K_G$  Growth kernel
  - $K_{Sk}$  Shrinkage kernel
  - 430 *M* Moment
  - N* Number
  - P** Symmetric tridiagonal matrix as a function of recursion coefficients  $a$  and  $b$
  - P* Fragment distribution function
  - R* Source term due to inception
  - S* Source term due to shrinkage
  - V** Eigenvalues of matrix **P**
  - W* Source term due to growth
  - Z** Matrix with components  $Z$  which are a function of the moments
- M*

*Lower-case Roman*

$a, b$  Recursion coefficients

$h$  Time interval

$i$  particle mass class

$m$  Mass

$r$  Recursive function

$t$  Time

$w$  weight

*Greek*

431

$\alpha$  Particle mass

$\delta$  Particle mass change in a growth or shrinkage process

*Subscripts*

f Final

L Large

p Particle

0 Initial or zero

1 Smallest particle mass class

*Symbols*

- $\tilde{x}$  Approximation of  $x$
- $\hat{b}$  Integral of fragmentation distribution function

*Abbreviations*

- DQMOM Direct quadrature method of moments
- DSA Direct simulation algorithm
- EQMOM Extended quadrature method of moments
- FCMOM Finite-size domain complete set of trial functions method of mo-  
432 ments
- HMOM Hybrid method of moments
- MOM Method of moments
- MOMIC Method of moments with interpolative closure
- MPM Moment projection method
- ODE Ordinary differential equation
- PBE Population balance equation
- PSD Particle size distribution
- QMOM Quadrature method of moments

433 **Appendix A. Blumstein-Wheeler algorithm**

434 This algorithm is used to determine the particle masses and the numbers  
435 used to approximate the PSD from the empirical moments. The algorithm is  
436 implemented in Matlab and makes use of the eig function to determine the  
437 eigenvalues and eigenvectors.

---

**Algorithm 2:** Blumstein-Wheeler algorithm.

---

**Input:** The empirical moments  $\widetilde{M}_k$  for  $k = 0, 1, \dots, 2N_p - 2$ .

**Output:** The particle masses  $\alpha_j$  and the corresponding number of particles  $\widetilde{N}_{\alpha_j}$  for  $j = 1, 2, \dots, N_p$ .

Create a  $N_p \times 2N_p$  matrix  $\mathbf{Z}$  with zeros in all elements.

Determine the elements of the first row of matrix  $\mathbf{Z}$ :  $Z_{1,l} = \widetilde{M}_{l-1}$  for  $l = 1, \dots, 2N_p - 1$ .

For  $a_1 = \widetilde{M}_1/\widetilde{M}_0$  and  $b_1 = 0$ , determine the recursion coefficients  $a_k$  and  $b_k$ :

**for**  $k = 2$  to  $N_p$  **do**

**for**  $l = k$  to  $2N_p - 1$  **do**

        The elements of  $\mathbf{Z}$  must satisfy the following recursion relation:

$$Z_{k,l} = Z_{k-1,l+1} - a_{k-1}Z_{k-1,l} - b_{k-1}Z_{k-1,l};$$

$$a_k = \frac{Z_{k,k+1}}{Z_{k,k}} - \frac{Z_{k-1,k}}{Z_{k-1,k-1}}; \quad b_k = \frac{Z_{k,k}}{Z_{k-1,k-1}}.$$

For  $r_1 = 1/(m_1 - a_1)$  where  $m_1$  is the smallest particle mass, determine the recursion function:

$$r_k = 1/(m_1 - a_k - b_k r_{k-1}), \quad k = 2, \dots, N_p - 1.$$

As we fix the smallest particle mass, replace  $a_{N_p}$  with:

$$a_{N_p} = m_1 - b_{N_p} r_{N_p-1}.$$

Construct a symmetric tridiagonal matrix  $\mathbf{P}$  with  $a_k$  as the diagonal and the square roots of  $b_k$  as the co-diagonal:

$$\mathbf{P} = \begin{bmatrix} a_1 & -\sqrt{b_2} & 0 & \cdots & 0 \\ -\sqrt{b_2} & a_2 & -\sqrt{b_3} & \cdots & 0 \\ 0 & -\sqrt{b_3} & a_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{N_p} \end{bmatrix}.$$

Solve for the eigenvalues  $\mathbf{V}$  and eigenvectors  $\mathbf{D}$  of matrix  $\mathbf{P}$ :

$$[\mathbf{V}, \mathbf{D}] = \text{eig}(\mathbf{P}).$$

Solve for  $\alpha_j$  and  $\widetilde{N}_{\alpha_j}$ :

$$\alpha_j = \mathbf{V}(j, j), \quad \widetilde{N}_{\alpha_j} = \widetilde{M}_0 \mathbf{D}(1, j)^2.$$


---

439 **Appendix B. Hybrid method of moments**

440 The hybrid method of moments (HMOM) was originally developed for  
 441 bivariate population balance equations (PBEs) based on particle volume and  
 442 surface area [6, 7]. Here we revise the method so that it is applicable to  
 443 monovariate PBEs. Below is a brief description of HMOM based on particle  
 444 mass for symmetric fragmentation with a constant kernel.

445 Following the idea in Ref. [6], the particles are discretised into two modes:  
 446 particles of the smallest mass class  $i_0$  and particles of the large mass class  $i_L$ .  
 447 The moments can then be represented as:

$$M_k = N_{i_0} i_0^k + N_{i_L} i_L^k, \quad (\text{B.1})$$

448 where  $N_{i_0}$  and  $N_{i_L}$  are the number of particles of mass  $i_0$  and  $i_L$ , respec-  
 449 tively. The fragmentation moment source term for symmetric fragmentation  
 450 with a constant kernel (Eq. (24)) can then be written as:

$$\frac{dM_k}{dt} = \begin{cases} K_{\text{Fg}} N_{i_L}, & k = 0, \\ 0, & k = 1, \\ (2^{1-k} - 1) K_{\text{Fg}} i_L^k N_{i_L}, & k > 1. \end{cases} \quad (\text{B.2})$$

451 The source term for  $N_{i_0}$  is given by the negative infinity order moments:

$$\frac{dN_{i_0}}{dt} = \lim_{k \rightarrow -\infty} \frac{dM_k/dt}{i_0^k}. \quad (\text{B.3})$$

452 Applying Eq. (B.3) to Eq. (6) for symmetric fragmentation, we obtain:

$$\frac{dN_{i_0}}{dt} = 2K_{\text{Fg}} N_{2i_0}. \quad (\text{B.4})$$



453 The only unknown term  $N_{2i_0}$  corresponds to the intermodal transfer of  
 454 particles from the second mode to the first during the fragmentation pro-  
 455 cess. To close this term, in Ref. [6] it is assumed that the rate of transfer  
 456 is proportional to the overall fragmentation rate with a coefficient equal to  
 457 the mass ratio between the two modes  $i_0/i_L$ . As a result, Eq. (B.4) can be  
 458 transformed into:

$$\frac{dN_{i_0}}{dt} = \frac{2i_0^2}{i_L^2} K_{\text{Fg}} N_{i_L}. \quad (\text{B.5})$$

459 assuming the remaining two quantities in Eq. (B.1) are obtained by in-  
 460 verting the system with two known moments:

$$N_{i_L} = M_0 - N_{i_0}, \quad (\text{B.6})$$

461 and

$$i_L = \frac{M_1 - N_{i_0} i_0}{N_{i_L}}. \quad (\text{B.7})$$

462 Algorithm 3 describes the numerical procedure of HMOM for symmetric  
 463 fragmentation with a constant kernel. HMOM for other processes (inception,  
 464 growth, shrinkage, coagulation, symmetric fragmentation with a mass-  
 465 dependent kernel, erosion fragmentation with a constant or mass-dependent  
 466 kernel) can be obtained in a similar way. The details are not given here for  
 467 simplicity.

---

**Algorithm 3:** Hybrid method of moments algorithm.

---

**Input:** PSD supplied as initial condition  $N(i, t_0)$  for  $i = 1, \dots, \infty$  at initial time  $t_0$ ; final time  $t_f$ .

**Output:** Moments  $M_k(t_f)$  for  $k = 0, 1, \dots$  at final time  $t_f$ .

Calculate the moments of the true PSD using Eq. (9):

$$M_k(t_0) = \sum_{i=1}^{\infty} i^k N(i, t_0), \quad k = 0, \dots, 2N_p - 2.$$

Determine the number and mass of the large particles  $N_{i_L}(t_0)$  and  $i_L(t_0)$ , respectively, by solving Eqs. (B.6) and (B.7).

$t \leftarrow t_0, M_k(t) \leftarrow M_k(t_0);$

**while**  $t < t_f$  **do**

Integrate Eq. (B.2) for the moments  $M_k(t+h)$  over the time interval  $[t, t+h]$  (using an ODE solver) with  $N_{i_0}(t)$ ,  $N_{i_L}(t)$  and  $i_L(t)$  as the initial condition.

Integrate Eq. (B.5) for the number of smallest particles  $N_{i_0}(t+h)$  over the time interval  $[t, t+h]$  with  $N_{i_0}(t)$ ,  $N_{i_L}(t)$  and  $i_L(t)$  as the initial condition.

Determine  $N_{i_L}(t+h)$  using Eq. (B.6) with the obtained  $M_0(t+h)$  and  $N_{i_0}(t+h)$ .

Determine  $i_L(t+h)$  using Eq. (B.7) with the obtained  $M_1(t+h)$ ,  $N_{i_0}(t+h)$  and  $N_{i_L}(t+h)$ .

Increment  $t \leftarrow t+h$ .

---

468

469 **Appendix C. Quadrature method of moments**

470 The quadrature method of moments (QMOM) used in this work is similar  
 471 to the one in Ref. [20]. This method was originally derived from continuous  
 472 PSD approaches. Here we give a simple description about the way QMOM  
 473 is used for fragmentation processes with a discrete-mass distribution.

474 In order to apply the QMOM, the fragmentation equation must first be  
 475 transformed into moment equation which is the same as Eq. (15):

$$\frac{dM_k}{dt} = \sum_{j=1}^{\infty} \sum_{i=1}^j K_{\text{Fg}}(j) i^k P(i|j) N_j - \sum_{i=1}^{\infty} K_{\text{Fg}}(i) i^k N_i. \quad (\text{C.1})$$

476 The QMOM is based on the following quadrature approximation:

$$M_k \approx \sum_{\alpha=1}^N i_{\alpha}^k w_{\alpha}, \quad (\text{C.2})$$

477 where  $N$  is the number of quadrature nodes.  $i_{\alpha}$  and  $w_{\alpha}$  are respectively the  
 478 quadrature abscissas and weights and their values can be determined using a  
 479 product-different (PD) algorithm from lower-order moments [53]. Applying  
 480 Eq. (C.2) to Eq. (C.1) leads to

$$\frac{dM_k}{dt} = \sum_{\alpha=1}^N K_{\text{Fg}}(i_{\alpha}) w_{\alpha} \widehat{b}(i_{\alpha}) - \sum_{\alpha=1}^N i_{\alpha}^k K_{\text{Fg}}(i_{\alpha}) w_{\alpha}, \quad (\text{C.3})$$

481 where

$$\widehat{b}(i_{\alpha}) = \sum_{i=1}^{i_{\alpha}} i^k P(i|i_{\alpha}). \quad (\text{C.4})$$

482 For symmetric fragmentation

$$\widehat{b}(i_\alpha) = 2^{1-k} i_\alpha^k, \quad (\text{C.5})$$

483 and for erosion

$$\widehat{b}(i_\alpha) = 1^k + (i_\alpha - 1)^k. \quad (\text{C.6})$$

484 Note that  $K_{\text{Fg}}(i_\alpha = 1) = 0$  since the smallest particles cannot fragment.

485 Algorithm 4 describes the numerical procedure of QMOM for fragmenta-  
 486 tion process. QMOM for other processes can be obtained in a similar way.

487 The details are not given here for simplicity.

---

**Algorithm 4:** Quadrature method of moments algorithm.

---

**Input:** PSD supplied as initial condition  $N(i, t_0)$  for  $i = 1, \dots, \infty$  at initial time  $t_0$ ; final time  $t_f$ .

**Output:** Moments  $M_k(t_f)$  for  $k = 0, 1, \dots$  at final time  $t_f$ .

Calculate the moments of the true PSD using Eq. (9):

$$M_k(t_0) = \sum_{i=1}^{\infty} i^k N(i, t_0), \quad k = 0, \dots, 2N - 1.$$

Determine the values of  $i_\alpha$  and  $w_\alpha$  ( $\alpha = 1, \dots, N$ ) based on the  $2N$  moments using the PD algorithm.

488

$t \leftarrow t_0$ ,  $M_k(t) \leftarrow M_k(t_0)$ ;

**while**  $t < t_f$  **do**

Integrate Eq. (C.3) for the moments  $M_k(t+h)$  over the time interval  $[t, t+h]$  (using an explicit Runge-Kuta method):

$$\frac{dM_k}{dt} = \sum_{\alpha=1}^N K_{\text{Fg}}(i_\alpha) w_\alpha \hat{b}(i_\alpha) - \sum_{\alpha=1}^N i_\alpha^k K_{\text{Fg}}(i_\alpha) w_\alpha,$$

with the quadrature abscissas and weights:  $i_\alpha, w_\alpha$  ( $\alpha = 1, \dots, N$ ).

Update  $i_\alpha$  and  $w_\alpha$  using the PD algorithm with the obtained  $M_k(t+h)$ .

Increment  $t \leftarrow t+h$ .

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