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## A novel finite-volume TVD scheme to overcome non-realizability problem in quadrature-based moment methods

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### Abstract

A new finite-volume total variation diminishing (TVD) scheme is proposed for the solution of moment transport equations in quadrature-based moment methods (QBMM). The proposed scheme is capable of preserving important properties of the moments, such as realizability and boundedness. The idea behind the approach is to limit the flux of all the moments at each cell face with the same limiter value. The proposed numerical technique was eventually compared with other realizable schemes developed for the moment transport equations, showing that the method is able to keep the moments realizable and bounded at the same time.

Keywords: Quadrature-based moment methods (QBMM); Moment

realizability; Moment boundedness; Population balance equation (PBE); High-resolution scheme; Finite-volume method.

1 1. Introduction

The evolution in space and time of a population of disperse elements (e.g., droplets, bubbles or particles moving in a continuous fluid) can be described by using an Eulerian approach through the solution of a generalized

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population balance equation (GPBE). It is an integro-differential equation 5 written in terms of a number density function (NDF) representing, at every 6 point of the physical space, the number of elements that have a particular 7 state belonging to the so-called phase space, i.e. the space of the properties 8 required to characterize the system under investigation (e.g. element size. 9 locity, chemical composition, temperature). The Quadrature-Based Moment 10 Methods (QBMM) are proved to be efficient in solving the GPBE, where the 11 transport equations for some moments of the underlying NDF are solved in-12 stead of the GPBE [1]. These methods are based on the assumption that the 13 underlying NDF has the form of a multi-dimensional summation of weighted 14 kernel density functions (KDF) centered on the quadrature abscissas, where 15 the quadrature weights and abscissas can be retrieved from the moments by 16 means of the so-called inversion algorithms (such as the Product-Difference 17 (PD) [2] and the Chebyshev [3] algorithms). In most cases, the KDF is a 18 Dirac delta function, especially when a continuous reconstruction of the NDF 10 is not necessary. While these methods are efficient and promising, especially 20 when coupled with Computational Fluid Dynamics (CFD) codes, their prac-21 tical use encounters inherent difficulties to cope with. One major issue is 22 the realizability or consistency of the transported moment set, meaning that 23 there must exist an underlying number density function (NDF) corresponding 24 to the transported moments. Confining the discussion to the finite-volume 25 method, the most common cause of the non-realizability (also known as nu-26 merical moment corruption) lies in the spatial discretization of the transport 27 term of the moment equation, when high-order spatial discretization schemes 28 are used. This problem is often related to the convective term, as in many 29

cases the governing equations have a hyperbolic form. Desjardins et al. [4] 30 demonstrated that the 1<sup>st</sup>-order scheme guarantees the realizability of the 31 moments, provided the CFL condition is respected. However, this scheme 32 results in highly diffusive solutions, leading sometimes to unacceptable pre-33 dictions, hence the necessity of adopting high-order schemes. On the other 34 hand, employing high-order finite-volume schemes for independent transport 35 of the moments may cause non-realizability issues [5]. Therefore, the devel-36 opment of a realizable high-order scheme for the solution of moment trans-37 port equations is crucial. In this regard, Vikas and co-workers [6] presented 38 the so-called realizable quasi-high-order schemes, based on the evaluation 39 of the moment fluxes at the cell faces using the interpolated abscissas and 40 weights of the quadrature. With this method, the quadrature interpola-41 tion is performed by applying 1<sup>st</sup>-order scheme to the quadrature abscissas 42 and high-order schemes to the quadrature weights. This approach produces 43 less diffusive solutions and guarantees the realizability of the transported 44 moments, provided a criterion on the time step is respected. However, no 45 analysis was conducted on the boundedness property of this approach, which 46 can not be ignored since unbounded predictions are not physically allowed 47 [7]. Kah et al. [8] formulated a 2<sup>nd</sup>-order kinetic scheme that makes use of 48 the canonical moments to transport the moments indirectly while maintain-49 ing them in the moment space. However, the application of their method 50 to simulations with more than four moments involves difficult algebra [9]. 51 Recently, Laurent and co-workers [9] developed a similar approach based on 52 reconstructing the coefficients  $\zeta_k$  (for its definition refer to [9]) instead of the 53 canonical moments. However, their original  $\zeta_k$  reconstruction based scheme 54

cannot be applied easily to the unstructured grids and therefore they suggested a simplified version of this scheme that involves division of the cells
into three parts as proposed by Berthon [10].

The present work introduces a new technique, called equal-limiter scheme, 58 to overcome the non-realizability problem when 2<sup>nd</sup>-order TVD (Total Vari-59 ation Diminishing) schemes are applied to the moment transport equations. 60 The technique is based on using an equal limiter given by the hux-limiter 61 function for all the moments, and it will be shown that it is effective to 62 avoid non-realizable set of moments. Moreover, its application to three-63 dimensional unstructured grids is straightforward. The paper is organized as 64 follows. First, it will be proved that, in a one-dimensional Riemann problem, 65 the concept of equal-limiter emerges naturally if no source term is included in 66 the moment transport equations. Next, the importance of using an identical 67 limiter given by the limiter function for all the moments will be clarified in 68 a general case by solving local Riemann problem at each cell face and the 60 role of the time step in maintaining the realizability of the moments will be 70 explained. Moreover, the paper shows how this technique can be applied to 71 CFD codes, without any assumption on velocity field or type of mesh grid. In 72 the final part, a comparison between different techniques will be performed 73 by solving moment transport equations in some one- and two-dimensional 74 test case 75

#### <sup>76</sup> 2. TVD scheme for moment transport equation

### 77 2.1. Moment transport equation

As previously mentioned, QBMM deal with the solution of the trans-78 port equations written in terms of the moments of the NDF, instead of the 79 GPBE itself. The NDF is a complex multi-dimensional functional that de-80 pends on the so-called external coordinates, i.e. the position of the elements 81 in the physical space and time, and on the internal coordinates, which are 82 the generic properties associated to each element of the population, such as 83 size, velocity, chemical composition or temperature. When the internal co-84 ordinates do not include the velocity of the elements of the disperse phase, 85 the resulting transport equation for the NDF is called Population Balance 86 Equation (PBE) [1]. Although it is possible to apply the proposed numerical 87 scheme to the transport equation for a multivariate set of moments, let us 88 consider a univariate PBE with the size of the elements of the disperse phase, 89 L, as the internal coordinate, for the sake of simplicity and clarity. In this 90 case, the PBE can be written as follows [11]:

$$\frac{\partial f}{\partial t} + \frac{\partial (\mathbf{U}f)}{\partial \mathbf{x}} + \frac{\partial (\dot{L}f)}{\partial L} = h \tag{1}$$

where  $f = f(L, \mathbf{x}, t)$  denotes the NDF. In addition,  $\mathbf{U} \equiv \mathbf{U}(\mathbf{x}, t)$  is the velocity of the disperse phase,  $\dot{L}$  represents the continuous rate of change in the size of elements due to the continuous processes (e.g. mass transfer driven growth) and h introduces the contribution of the discrete events (e.g. aggregation/breakage) into the PBE. It is worth remarking that the velocity of the disperse phase appearing in Eq. (1) does not depend on the size of the elements: such approximation has been made to simplify the following
discussion and it is not a limitation of the proposed approach.

By definition, the  $k^{\text{th}}$ -order moment of f with respect to L is:

$$M^{k}(\mathbf{x},t) = \int_{0}^{\infty} f(L,\mathbf{x},t) L^{k} dL$$

The importance of the moments lies in the fact that lower-order moments 101 are associated to various integral properties of the population. For instance, 102 in this case the  $3^{rd}$ -order moment with respect to L is proportional to the 103 volume fraction of the disperse phase. The above definition can be used to 104 derive moment transport equations from Eq.  $(1)_{\star}$  For the sake of simplicity, 105 from now on we assume a one-dimensional case where the velocity is constant 106 (u) and the contribution of the continuous processes is negligible  $(\dot{L} = 0)$ . 107 The transport equation for the  $k^{\text{th}}$  order moment reduces to the following 108 partial differential equation: 109

$$\frac{\partial M^k}{\partial t} + u \frac{\partial M^k}{\partial x} = \bar{h}^k \tag{3}$$

where  $\bar{h}^k$  is the source term changing the  $k^{\text{th}}$ -order moment due to the discrete events. Generally, this source term is a complex multi-dimensional integral which depends on the NDF itself. QBMM employ the so-called quadrature approximation to express the functional form of the NDF. If we consider only one internal coordinate, it is possible to write a generic integral in the following way and therefore close the moment transport equations:

$$\int_{\Omega_L} f(L)g(L)dL = \sum_{\alpha=1}^N w_\alpha g(L_\alpha) \tag{4}$$

where  $w_{\alpha}$  and  $L_{\alpha}$  are the weights and abscissas of the *N*-node quadrature formula. This means that the NDF is approximated as a summation of delta <sup>118</sup> functions centered on quadrature abscissas:

$$f(L) = \sum_{\alpha=1}^{N} w_{\alpha} \delta(L - L_{\alpha})$$
(5)

This method is called Quadrature Method of Moments (QMOM) and it is 119 designed to solve univariate PBE [12]. The weights and abscissas are deter-120 mined from the transported moments by employing an inversion algorithm 121 (such as PD or Chebyshev algorithms), provided the set of moments is re-122 alizable. This is usually referred as the moment problem [13]: in particular, 123 when the support of the NDF is  $\Omega_L = ]0, +\infty[$  as in this case, it is called 124 finite Stieltjes moment problem. When the support of the NDF is different, 125 i.e.  $\Omega_L = ]-\infty, +\infty [$  or  $\Omega_L = ]0, 1[$ , we refer to finite Hamburger and finite 126 Hausdorff moment problems respectively. These three different supports re-127 sult in different constraints on the transported set of moments to ensure 128 its realizability [13, 14]. However, the non-realizability problem is common 129 to all these cases and poses the main challenge in practical applications of 130 QMOM. In the finite-volume method, this can happen particularly during 131 the interpolation of the moments on to the faces to calculate the flux of the 132 moments through faces if high-resolution TVD schemes are employed. 133

## 134 2.2. Finite-Volume Method

As mentioned before, the present study focuses on the non-realizability issue in the context of the finite-volume method. The general formulation of the finite-volume method can be found in the specialized literature [15, 16], and therefore is omitted here. Let a single-stage explicit method be adopted to march in time and the source terms be handled using fractionalstep approach [15]. In this way, the finite-volume method transforms Eq. (3) into the following discretized form written for the generic cell i of size  $\Delta x$  in the spatial domain:

$$M_{i}^{k*} = M_{i}^{k} - \frac{\Delta t}{\Delta x} (F_{i+1/2}^{k} - F_{i-1/2}^{k})$$

$$(M_{i}^{k})^{n+1} = M_{i}^{k*} - \Delta t \ \bar{h}_{i}^{k}$$
(6)

where  $M_i^k$ ,  $M_i^{k*}$  and  $(M_i^k)^{n+1}$  refer to, respectively, the moment value at the 143 current time  $(t_n)$ , the intermediate value of the fractional-step approach and 144 the moment value at the new time  $(t_{n+1})$  after a time step of  $\Delta t$ . Further-145 more,  $F_{i-1/2}^k$  and  $F_{i+1/2}^k$  denote the numerical flux along the left and right 146 faces of the cell i respectively, each depends on the neighboring cell values at 147 time  $t_n$  according to the selected numerical flux function. From now on, the 148 primary focus of the work will be on Eq. (6), particularly the calculation of 149 the flux of the moments at the faces. The effect of the source term will be 150 clarified afterwards. 151

It is desirable to calculate the fluxes using high-resolution schemes, which 152 are on the basis of slope-limiter methods. These methods use a high-order 153 scheme where the solution is smooth enough, otherwise they switch to a low-154 order one to prevent non-physical oscillations in the numerical solution [15]. 155 In this way, the solution exhibits higher order of accuracy, comparing to 1<sup>st</sup>-156 order solution, without losing the boundedness. Using Lax-Wendroff as the 157 high-order scheme and upwind as the low-order one will form the so-called 158 flux-limiter methods with the following numerical flux functions [15]: 159

$$F_{i-1/2}^{k} = u^{-}M_{i}^{k} + u^{+}M_{i-1}^{k} + \frac{1}{2}|u| \left(1 - \frac{|u|\Delta t}{\Delta x}\right)\phi(\theta_{i-1/2}^{k})\Delta M_{i-1/2}^{k}$$
(8)

$$F_{i+1/2}^{k} = u^{-}M_{i+1}^{k} + u^{+}M_{i}^{k} + \frac{1}{2}|u| \left(1 - \frac{|u|\Delta t}{\Delta x}\right)\phi(\theta_{i+1/2}^{k})\Delta M_{i+1/2}^{k}$$
(9)

160 where

$$u^{+} = \frac{1}{2}(u + |u|)$$
 and  $u^{-} = \frac{1}{2}(u - |u|)$  (10)

In addition,  $\Delta M_{i-1/2}^k$  and  $\Delta M_{i+1/2}^k$  are respectively the jumps across the left and right faces, defined following the below convention:

$$\Delta M_{i-1/2}^{k} = M_{i}^{k} - M_{i-1}^{k}$$

<sup>163</sup> The flux-limiter  $\phi$  is a function of the smoothness of  $M^k$  at the face  $(\theta_{i\pm 1/2}^k)$ . <sup>164</sup> The smoothness is commonly defined as follows [15]:

$$\theta_{i-1/2}^{k} = \frac{\Delta M_{I-1/2}^{k}}{\Delta M_{i-1/2}^{k}} \quad \text{with} \quad I = \begin{cases} i-1 & \text{if } u > 0\\ i+1 & \text{if } u < 0 \end{cases}$$
(12)

A variety of flux-limiter functions are available in the literature such as minmod [17] and van Leer [18].

<sup>167</sup> Substituting the numerical fluxes in Eq. (6) yields the following dis-<sup>168</sup> cretized equation:

$$M_{i}^{k*} = M_{i}^{k} - \Delta t = (M_{i}^{k} - M_{i-1}^{k}) - \frac{\Delta t}{\Delta x} u^{-} (M_{i+1}^{k} - M_{i}^{k})$$

$$\frac{1}{2} \Delta x \left(1 - \frac{|u|\Delta t}{\Delta x}\right) \left[\phi(\theta_{i+1/2}^{k})\Delta M_{i+1/2}^{k} - \phi(\theta_{i-1/2}^{k})\Delta M_{i-1/2}^{k}\right]$$
(13)

<sup>169</sup> 3. The Concept of Equal-Limiter

The flux-limiter methods were developed to address the issue of boundedness that occurs in the case of employing high-order schemes to solve hyperbolic problems. One would ideally desire to use these methods for the solution of the moment transport equations, particularly when the 1<sup>st</sup>-order accuracy is not sufficient to describe the behavior of the system under study.
However, in general, the non-realizability problem hinders their direct practice in solving the moments transport equations. In this section, it is shown
that this limitation can be overcome by selecting an equal limiter for all the
moments.

The starting point is to show that the idea of equal-limiter emerges in the case of employing 2<sup>nd</sup>-order TVD schemes for the pure moment advection with no source term  $((M_i^k)^{n+1} = M_i^{k*})$  in a Riemann problem) example. It will be also shown that in this case the moments remain realizable. Then, the discussion will continue to highlight the advantage of employing equal-limiter in a more general context, where the effect of aggregation and breakage will be also taken into account.

The argument begins with rewriting Eq. (13) for the case u > 0 without loss of generality<sup>1</sup>:

$$(M_{i}^{k})^{n+1} = M_{i}^{k} - \nu (M_{i}^{k} - M_{i-1}^{k}) - \frac{1}{2} \nu (1 - \nu) \left[ \phi(\theta_{i+1/2}^{k}) \Delta M_{i+1/2}^{k} - \phi(\theta_{i-1/2}^{k}) \Delta M_{i-1/2}^{k} \right]$$
(14)

where  $\nu = u\Delta t/\Delta x$  is the Courant number. The smoothness at the left and right faces are written as follows Eq. (12):

$$\theta_{i-1/2}^{k} = \frac{M_{i-1}^{k} - M_{i-2}^{k}}{M_{i}^{k} - M_{i-1}^{k}} \quad \text{and} \quad \theta_{i+1/2}^{k} = \frac{M_{i}^{k} - M_{i-1}^{k}}{M_{i+1}^{k} - M_{i}^{k}}$$
(15)

<sup>190</sup> Now let us consider a Riemann problem example with the following initial

<sup>&</sup>lt;sup>1</sup>The case u < 0 can be formulated similarly and leads to the same conclusions

191 data:

$$M^{k}(x,0) = \overset{\circ}{M^{k}}_{l} = \begin{cases} \overset{\circ}{M^{k}_{l}} & \text{if } x < 0\\ \circ\\ M^{k}_{r} & \text{if } x > 0 \end{cases}$$
(16)

where  $M_l^k$  and  $M_r^k$  are obtained from the initial left and right NDFs,  $f_l$  and  $f_r$ , and consequently constitute two realizable sets of moments. It is postulated that the numerical solution of the  $k^{\text{th}}$ -order moment at any generic cell *i* and any time step  $t_n$ , including the zero time, can be expressed as:

$$M_{i}^{k} = \mathring{M}_{r}^{k} - a_{i}^{n}(\mathring{M}_{r}^{k} - \mathring{M}_{l}^{k}) \quad , \quad 0 \le a_{i}^{n} \le 1$$
(17)

where  $a_i^n$  is a constant that changes with the cell index *i* and the time step but not due to the moment order or value. In other words, this constant is the same for all the moments of a given cell at each time step. It is worth mentioning that the initial data (Eq. (16)) corresponds to  $a_i^0 = 1$  for  $x_i < 0$ and  $a_i^0 = 0$  for  $x_i > 0$ . Next step is to substitute Eq. (17) in Eq. (14), which after simplifications yields the following:

$$(M_{i}^{k})^{n+1} = M_{r}^{k} - a_{i}^{n}(M_{r}^{k} - M_{l}^{k}) + \nu(a_{i}^{n} - a_{i-1}^{n})(M_{r}^{k} - M_{l}^{k}) + \frac{1}{2}\nu(1-\nu) \left[ \phi\left(\frac{a_{i}^{n} - a_{i-1}^{n}}{a_{i+1}^{n} - a_{i}^{n}}\right)(a_{i+1}^{n} - a_{i}^{n}) - \phi\left(\frac{a_{i-1}^{n} - a_{i-2}^{n}}{a_{i}^{n} - a_{i-1}^{n}}\right)(a_{i}^{n} - a_{i-1}^{n}) \right] (M_{r}^{k} - M_{l}^{k}) = M_{r}^{k} - a_{i}^{n+1}(M_{r}^{k} - M_{l}^{k})$$

$$(18)$$

202 and  $a_i^{n+1}$  collects several coefficients that do not depend on the moment

203 values:

$$a_{i}^{n+1} = a_{i}^{n} - \nu(a_{i}^{n} - a_{i-1}^{n}) - \frac{1}{2}\nu(1-\nu) \left[ \phi\left(\frac{a_{i}^{n} - a_{i-1}^{n}}{a_{i+1}^{n} - a_{i}^{n}}\right) (a_{i+1}^{n} - a_{i}^{n}) - \phi\left(\frac{a_{i-1}^{n} - a_{i-2}^{n}}{a_{i}^{n} - a_{i-1}^{n}}\right) (a_{i}^{n} - a_{i-1}^{n}) \right]$$
(19)

Equation (19) has the same structure of Eq. (14), therefore, it appears that  $a_i^n$  is the solution of an advection equation for the variable *a* obtained by the  $2^{nd}$ -order TVD finite-volume scheme. As a consequence, it is guaranteed that  $a_i^{n+1}$  remains bounded to the values of the previous time step, i.e. between 0 and 1. Now it can be concluded that the postulated solution at time step  $t_n$  is also valid at the next time step  $t_{n+1}$ :

$$(M_i^k)^{n+1} = \overset{\circ}{M_r^k} - a_i^{n+1} (\overset{\circ}{M_r^k} - \overset{\circ}{M_i^k}), \quad 0 \le a_i^{n+1} \le 1$$
(20)

As mentioned before, the initial data (Eq. (16)) can be expressed by Eq. (17), therefore, the postulated solution is indeed the solution of Eq. (14) at any time step with the initial data defined by Eq. (16). Moreover, it can be proved that the solution guarantees the realizability of the moments at any time step if the initial set is realizable. To proceed with the proof, the following notation is used for representing the set of moments:

$$\mathbf{W} = \begin{bmatrix} M^0 & M^1 & \dots & M^{2N-1} \end{bmatrix}^T$$
(21)

It is worth reiterating that N is the number of quadrature nodes. The set of moments can be defined as follows:

$$\mathbf{W} = \int_0^\infty f(L)\mathbf{q}(L)dL \tag{22}$$

where  $\mathbf{q}(L) = \begin{bmatrix} L^0 & L^1 & \dots & L^{2N-1} \end{bmatrix}^T$ .

Equation (20) can be written for the set of moments by using the notation introduced in Eq. (21):

$$\mathbf{W}_{i}^{n+1} = \mathbf{W}_{r} - a_{i}^{n+1}(\mathbf{W}_{r} - \mathbf{W}_{l})$$
It should be emphasized that Eq. (23) is derived based on the fact that  $a_{i}^{n+1}$ 
is identical for all the moments. The proof follows by substituting Eq. (22)

<sup>223</sup> in Eq. (23) and performing some manipulations:

$$\int_{0}^{\infty} f_{i}^{n+1} \mathbf{q}(L) dL = \int_{0}^{\infty} [(1 - a_{i}^{n+1}) \mathring{f}_{r} + a_{i}^{n+1} \mathring{f}_{t}] \mathbf{q}(L) dL$$
(24)

224 Or

221

222

$$f_i^{n+1} = (1 - a_i^{n+1}) \mathring{f}_r + a_i^{n+1} \mathring{f}_l$$
(25)

The above equation guarantees the non-negativity of the  $f_i^{n+1}$  because both  $\stackrel{\circ}{f_r}$  and  $\stackrel{\circ}{f_l}$  are defined to be non-negative NDFs and  $0 \le a_i^{n+1} \le 1$ . Consequently, the moment set of cell *i* at time step  $t_{n+1}$  is realizable, see [4].

Returning back to the equal-limiter concept, it was previously highlighted that an identical  $a_i^{n+1}$  for all the moments is essential to keep the moment set realizable in a Riemann problem example. The identical  $a_i^{n+1}$  originates, in turn, from the equal limiters calculated at the left and right faces (i.e., Eq. (18)):

$$\phi(\theta_{i-1/2}^k) = \phi\left(\frac{a_{i-1}^n - a_{i-2}^n}{a_i^n - a_{i-1}^n}\right) \quad \text{and} \quad \phi(\theta_{i+1/2}^k) = \phi\left(\frac{a_i^n - a_{i-1}^n}{a_{i+1}^n - a_i^n}\right).$$
(26)

<sup>233</sup> When source terms are present, the limiters are not generally identical for <sup>234</sup> all the moments, because in this case the smoothness of the moments may change differently and this may cause the non-realizability of the transported
moment set. This suggests to find a technique to employ an identical limiter
in the calculation of the moment fluxes at the faces.

Again Eq. (13) is rewritten for the case of u > 0 (here a local Riemann problem is solved at each face of cell *i*):

$$M_{i}^{k*} = M_{i}^{k} - \nu (M_{i}^{k} - M_{i-1}^{k}) - \frac{1}{2} \nu (1 - \nu) [\phi(\theta_{i+1/2}^{k}) \Delta M_{i+1/2}^{k} - \phi(\theta_{i-1/2}^{k}) \Delta M_{i-1/2}^{k}]$$
(27)

which can simply be expressed as follows by collecting the terms containing the moment of cells i - 1, i and i + 1:

$$M_i^{k*} = B_i^k M_{i-1}^k + C_i^k M_i^k - D_i^k M_{i+1}^k$$
(28)

242 with

$$B_{i}^{k} = \nu - \frac{1}{2}\nu(1-\nu)\phi(\theta_{i+1/2}^{k})$$

$$C_{i}^{k} = 1 - \nu + \frac{1}{2}\nu(1-\nu)(\phi(\theta_{i+1/2}^{k}) + \phi(\theta_{i-1/2}^{k}))]$$

$$D_{i}^{k} = \frac{1}{2}\nu(1-\nu)\phi(\theta_{i+1/2}^{k})$$
(29)

<sup>243</sup> Writing Eq. (28) for the set of moments of order k = 1, 2, ..., 2N - 1 yields:

$$\begin{pmatrix} M_{i}^{0*} \\ M_{i}^{1*} \\ \vdots \\ M_{i}^{2N-1*} \end{pmatrix} = \underbrace{\begin{pmatrix} B_{i}^{0}M_{i-1}^{0} \\ B_{i}^{1}M_{i-1}^{1} \\ \vdots \\ B_{i}^{2N-1}M_{i-1}^{2N-1} \end{pmatrix}}_{\text{set i-1}} + \underbrace{\begin{pmatrix} C_{i}^{0}M_{i}^{0} \\ C_{i}^{1}M_{i}^{1} \\ \vdots \\ C_{i}^{2N-1}M_{i}^{2N-1} \end{pmatrix}}_{\text{set i}} - \underbrace{\begin{pmatrix} D_{i}^{0}M_{i+1}^{0} \\ D_{i}^{1}M_{i+1}^{1} \\ \vdots \\ D_{i}^{2N-1}M_{i+1}^{2N-1} \end{pmatrix}}_{\text{set i+1}}$$
(30)

The three sets of moments in Eq. (30) can easily become non-realizable because, in general, the coefficients  $B_i^k$  as well as  $C_i^k$  and  $D_i^k$  might differ from one moment to another (belonging to the same moment set) as a consequence of unequal limiters. Marchisio and Fox [1] showed that a small change in just one moment can make a consistent set of moments non-realizable. On the other hand, if identical limiters are selected to estimate the fluxes of all the moments at the left and right faces, Eq. (30) can be written as follows:

$$\int_{0}^{\infty} f_{i}^{*} \mathbf{q}(L) dL = \int_{0}^{\infty} (B_{i} f_{i-1} + C_{i} f_{i} - D_{i} f_{i+1}) \mathbf{q}(L) dL$$
(31)

251 OT

$$f_i^* = B_i f_{i-1} + C_i f_i - D_i f_{i+1}$$
(32)

where  $B_i$  as well as  $C_i$  and  $D_i$  are defined below by choosing an equal limiter at the left face,  $\phi(\theta_{i-1/2})$ , and one at the right face,  $\phi(\theta_{i+1/2})$ , for all the moments:

$$B_{i} = \nu - \frac{1}{2}\nu(1-\nu)\phi(\theta_{i-1/2})$$

$$C_{i} = 1 - \nu + \frac{1}{2}\nu(1-\nu)[\phi(\theta_{i+1/2}) + \phi(\theta_{i-1/2})]$$

$$D_{i} = \frac{1}{2}\nu(1-\nu)\phi(\theta_{i+1/2})$$
(33)

It should be noted that there is still no proof for the moment realizability in the case of employing equal limiters when source terms in the moment transport equation are present, because the last term in Eq. (32) is negative [4] [6]. However, the contribution of the negative term can be kept small enough through adjusting the time step since the coefficient  $D_i$  diminishes as the time step is reduced to zero. In other words, the non-realizability problem

can be prevented by adjusting the time step, whereas it can arise easily 261 regardless of the time step if the limiters are calculated independently. One 262 should be careful when the moment sets lie on the boundary of the moment 263 space. In such case, the underlying number density functions are indeed 264 some point distributions, i.e summation of some weighted delta functions. 265 Therefore, if the moment sets in Eq. (30) are near or on the boundary of the 266 moment space, reduction of the time step cannot resolve the realizability issue 267 since the supports of the corresponding underlying number density functions 268 in Eq. (32) may hardly match each other. A possible remedy can be adopting 269 the 1-D adaptive quadrature technique proposed by Yuan and co-workers [19]. 270 By this technique, the maximum number of quadrature nodes is selected in 271 such a way that the moments required to calculate the quadrature weights 272 and abscissas form a set which is located in the interior of the moment space. 273 It is noteworthy that the local reduction of the number of quadrature nodes 274 is not a problem for the equal-limiter scheme, in contrast to the quasi-high-275 order scheme, since the variables to be interpolated are the moments and not 276 the quadrature abscissas and weights. 277

The final point to be addressed is the choice of an equal flux-limiter at 278 each face. In fact, the constraint on the boundedness of the solution narrows 279 the choice of the equal flux-limiter. As mentioned before, the 2<sup>nd</sup>-order TVD 280 schemes have this notable feature of preserving the solution bounded. It is 281 extremely useful for the QMOM since the low-order moments are propor-282 tional to physical properties that are bounded in nature, such as mean size, 283 surface area or volume fraction. Harten [20] established the sufficient crite-284 ria for a scheme to be TVD, which provide constraints on the flux-limiter 285

286 functions:

$$\phi(\theta) = 0$$
 if  $\theta < 0$  and  $0 \le \phi(\theta) \le \min(2\theta, 2)$  if  $\theta \ge 0$  (34)

Fig. 1 represents these constraints graphically (shaded area) following the work of Sweby [21]. Moreover, it depicts the 2<sup>nd</sup>-order region proposed by Sweby [21] (hatched area) within which the flux-limiter functions lie. Two such examples are shown by the solid line (minmod limiter [17]) and the dashed line (van Leer limiter [18]).

The flux-limiter functions in the literature share the common feature of being non-decreasing functions of  $\theta$ . Using this feature, it is simple to show that the smallest flux-limiter among all the limiters of the moments is an obvious choice that guarantees the boundedness of all the moments. The flux-limiters calculated independently by a general limiter function at a given face, e, can be represented as  $\phi(\theta_e^k)$  with k = 0, 1, ..., 2N - 1. These limiters respect the conditions expressed in Eq. (34):

$$\phi(\theta_e^k) = 0 \quad \text{if} \quad \theta_e^k < 0 \quad \text{and} \quad 0 \le \phi(\theta_e^k) \le \min(2\theta_e^k, 2) \quad \text{if} \quad \theta_e^k \ge 0 \tag{35}$$

<sup>299</sup> Suppose that  $\phi_{\sigma}^{\min}$  denotes the limiter with the minimum value:

$$\min_{e} \phi(\theta_e^m) \le \phi(\theta_e^k) \quad \text{for} \quad k = 0, 1, ..., 2N - 1$$
(36)

300 where

$$\theta_{e}^{m} \in \{\theta_{e}^{k} \mid k \in \{0, 1, ..., 2N - 1\}\}$$
(37)

<sup>301</sup> and since the flux-limiter functions are non-decreasing:

$$\theta_e^m \le \theta_e^k \quad \text{for} \quad k = 0, 1, \dots, 2N - 1 \tag{38}$$

On the other hand, the upper boundary of the TVD region shown in Eq. (35), min $(2\theta_e^k, 2)$ , is a non-decreasing function, therefore:

$$\min(2\theta_e^m, 2) \le \min(2\theta_e^k, 2) \quad \text{for} \quad k = 0, 1, ..., 2N - 1$$
(39)

since  $\phi_e^{\min}$  respects the conditions specified in Eq. (35), it can be concluded that:

$$0 \le \phi_e^{\min} \le \min(2\theta_e^k, 2) \quad \text{for} \quad k = 0, 1, ..., 2N - 1$$
 (40)

<sup>306</sup> in other words,  $\phi_e^{\min}$  falls always in the TVD region specified in Fig. 1 for all <sup>307</sup> the moments. As a result, the moments remain bounded using this limiter, <sup>308</sup> following the proof given by Harten [20].

It should be mentioned that, in general, the minimum limiter can fall outside the 2<sup>nd</sup>-order region of Sweby for some moments, hence resulting in solutions with accuracy of lower order. Nevertheless, the numerical results reported in the next section show remarkable improvements in comparison to the 1<sup>st</sup>-order solutions. More importantly, the results indicate a significant advantage of the proposed scheme over the realizable high-order scheme of Vikas et al. [6] since it is able to produce bounded solutions.

## 316 4. Application to CFD Codes

This section focuses on the application of the equal-limiter scheme to CFD codes, which is indeed our ultimate goal of introducing this scheme. For this purpose, the following three-dimensional conservative transport equation is considered for the  $k^{\text{th}}$ -order moment:

$$\frac{\partial M^k}{\partial t} + \frac{\partial}{\partial \mathbf{x}} \cdot (\mathbf{u}M^k) = 0 \tag{41}$$

The source term is not included since the focus is only on the advection of the moments. In the context of finite volume methods, Eq. (41) is integrated over the volume of each computational cell and then the integral of the convective term over the volume of each cell is replaced with the net flux of the moment through the faces of that cell (Gauss's theorem). Therefore, the following semi-discretized equation is obtained for a generic cell i [16]:

$$\frac{\mathrm{d}M_i^k}{\mathrm{d}t} + \frac{1}{\Delta V_i} \sum_e (\mathbf{u}_e \cdot \hat{\mathbf{n}}_e) S_e M_e^k = 0 \tag{42}$$

where  $M_e^k$  and  $\mathbf{u}_e$  are the moment of order k and the velocity at a generic 327 face e of cell i respectively. In addition,  $\hat{\mathbf{n}}_e$  and  $S_e$  denote respectively the 328 outward unit normal vector and the surface area of face e and  $\Delta V_i$  is the 329 volume of the cell i. The transient term in Eq. (42) is not discretized for the 330 reason that becomes clear later. In CFD codes, the flux of the velocity field 331 at the cell faces, i.e.  $(\mathbf{u}_e \cdot \hat{\mathbf{n}}_e) S_{ee}$  is generally known. However, the value of 332 the moments at the faces  $M_e$  is not available and should be interpolated 333 from the values at the centers of neighbouring cells. 334

The implementation of high-resolution TVD schemes in CFD codes is usually on the basis of central-difference scheme, of which the anti-diffusive contribution is limited to prevent oscillations in the solution [22]:

where  $M_{\rm U}^k$  and  $M_{\rm D}^k$  refer to the values of the moment of order k at the centers of the upwind and downwind cell neighbours of the face e respectively. The selection of the upwind and downwind cells is based on the direction of the velocity field at face e, which is the same for all the moments. In addition, the coefficient  $\lambda_e$  takes a positive constant value between 0 and 0.5, which depends on the distances between the center of face e and the centers of the two neighbouring cells. The advantage of employing an identical limiter can be illustrated by rearranging Eq. (43) and writing it for a set of 2N – moments as follows:

$$\begin{pmatrix}
M_{e}^{0} \\
M_{e}^{1} \\
\vdots \\
M_{e}^{2N-1} \\
\vdots \\
M_{e}^{2N-1}
\end{pmatrix} = \left( \begin{array}{c}
\left[1 - \lambda_{e}\phi(\theta_{e}^{0})\right]M_{U}^{0} \\
\left[1 - \lambda_{e}\phi(\theta_{e}^{1})\right]M_{U}^{1} \\
\vdots \\
\left[1 - \lambda_{e}\phi(\theta_{e}^{2N-1})\right]M_{U}^{2N-1}
\end{array} \right) + \left(\begin{array}{c}
\lambda_{e}\phi(\theta_{e}^{0})M_{D}^{0} \\
\lambda_{e}\phi(\theta_{e}^{1})M_{D}^{1} \\
\vdots \\
\lambda_{e}\phi(\theta_{e}^{2N-1})M_{D}^{2N-1}
\end{array} \right) \\
set U \qquad set D$$

$$(44)$$

In general, the limiters for different moments,  $\phi(\theta_e^0), \phi(\theta_e^1), \ldots, \phi(\theta_e^{2N-1})$  are not the same. Therefore, the moment sets "U" and "D" can easily become non-realizable, leading to the non-realizable set of interpolated moments at face *e*. However, selecting an identical limiter, let it be  $\phi_e^{\min}$ , guarantees the realizability of the interpolated moment set *e*, as long as the moment sets "U" and "D" are realizable:

$$\begin{pmatrix}
M_e^0 \\
M_e^1 \\
\vdots \\
M_e^{2N-1} \\
&\text{set e}
\end{pmatrix} = (1 - \lambda_e \phi_e^{\min}) \begin{pmatrix}
M_U^0 \\
M_U^1 \\
\vdots \\
M_U^{2N-1} \\
&\text{set U}
\end{pmatrix} + \lambda_e \phi_e^{\min} \begin{pmatrix}
M_D^0 \\
M_D^1 \\
\vdots \\
M_D^{2N-1} \\
&\text{set D}
\end{pmatrix}$$
(45)

It is worth reiterating that the value of limiter  $\phi_e^{\min}$  is between 0 and 2. Moreover, the moment sets "U" and "D" belong to the previous time step if an explicit method is used to advance in time, and therefore they are <sup>356</sup> realizable.

It should be noted that the realizability of the interpolated moments on the faces does not ensure the realizability of the calculated moments at the new time step. To elaborate, let the transient term in Eq. (42) be integrated using an explicit Euler scheme [16] and then write the fully-discretized equation for the set of 2N - 1 moments:

$$\mathbf{W}_{i}^{n+1} = \mathbf{W}_{i}^{n} - \frac{\Delta t}{\Delta V_{i}} \sum_{e} (\mathbf{u}_{e}^{n} \cdot \hat{\mathbf{n}}_{e}) S_{e} \mathbf{W}_{e}^{n}$$
(46)

The use of an identical limiter for all the moments guarantees that the moment set  $\mathbf{W}_{e}^{n}$  be realizable, and therefore an underlying number density function  $(f_{e}^{n})$  can be associated to it. This allows writing Eq. (46) as:

$$f_i^{n+1} = f_i^n - \frac{\Delta t}{\Delta V_i} \sum_e (\mathbf{u}_e^n \cdot \hat{\mathbf{n}}_e) S_e f_e^n$$
(47)

The summation in the above equation can be separated into two contributions of in-going and out-going fluxes:

$$f_i^{n+1} = f_i^n - \underbrace{\Delta t}_{i e} \min[(\mathbf{u}_e^n \cdot \hat{\mathbf{n}}_e), 0] S_e f_e^n}_{\text{in-going fluxes}} - \underbrace{\frac{\Delta t}{\Delta V_i} \sum_{e} \max[(\mathbf{u}_e^n \cdot \hat{\mathbf{n}}_e), 0] S_e f_e^n}_{\text{out-going fluxes}}$$
(48)

The in-going fluxes have positive sign and cannot rise the realizability issue, whereas, the outgoing fluxes have negative sign and can cause realizability issue, i.e. negativity of  $f_i^{n+1}$ . However, the out-going fluxes can be still decomposed into two separate upwind and downwind contributions corresponding to the upwind and downwind neighbouring cells of the corresponding faces. It is noteworthy that the upwind cell of these faces indeed coincides with cell i since the flux at these faces is out-going. Thus, the first and third terms of the RHS of Eq. (48) can be written as follows:

$$\left(1 - (1 - \lambda_e \phi_e^{\min}) \frac{\Delta t}{\Delta V_i} \sum_e \max[(\mathbf{u}_e^n \cdot \hat{\mathbf{n}}_e), 0] S_e\right) f_i^n - (1 - \lambda_e \phi_e^{\min}) \frac{\Delta t}{\Delta V_i} \sum_e \max[(\mathbf{u}_e^n \cdot \hat{\mathbf{n}}_e), 0] S_e f_{D_e}^n$$
(49)

where  $f_{D_e}^n$  denotes the (downwind) neighbouring cell separated by face e from cell *i*. As can be seen, the entire contribution of the cell *i* is positive as long as the coefficient behind  $f_i^n$  is positive, leading to the following CFL-like condition:

$$\frac{\Delta t}{\Delta V_i} \sum_{e} \max[(\mathbf{u}_e^n \cdot \hat{\mathbf{n}}_e), 0] S_e < 1$$
(50)

Therefore, the only remaining negative contributions are due to the infor-379 mation (distributions) of the downwind cells (with respect to cell i) that 380 propagates back into cell *i*, which is the characteristic of high-order schemes. 381 These negative contributions can generally lead to the non-realizability issue, 382 i.e. negativity of  $f_i^{n+1}$ . However, similar to the previous discussion done for 383 one-dimensional constant-velocity cases, the negative contributions can be 384 kept small (in comparison to the contribution of  $f_i^n$ ) by controlling the time 385 step. It is noteworthy that this technique may fail as the moment sets are 386 near/at the boundary of the moment space, as explained before. 387

Returning back to the time-integration of the transient term in Eq. (42), it should be noted that one notable advantage of the equal-limiter scheme is the possibility of using implicit time-integration for the advection of the moments. This is due the fact that the equal-limiter scheme interpolates the moments directly, whereas, for instance, the quasi-high-order scheme is <sup>393</sup> normally implemented using explicit time-integration schemes. This aspect
<sup>394</sup> is particularly important when the solution of the population balance equa<sup>395</sup> tion is incorporated into a CFD solver, since the implicit time-integration
<sup>396</sup> schemes are commonly adopted in these codes.

Lastly, the proposed technique is very simple from the computational point of view and can be easily implemented in three-dimensional CFD solvers. The only additional steps are comparing the limiter values calculated for the moments at each face and then replacing them with the smallest one at the corresponding face.

### 402 5. Numerical Examples

This section evaluates the performance of the proposed technique for the advection of moments in two different parts. The first one is focused on comparing the predictions obtained by different schemes for the advection of the moments in a mono-dimensional constant-velocity problem. The second part evaluates the performance of the schemes by solving the moment transport equations coupled with the CFD simulation of a two-dimensional transient lid-driven cavity flow.

### 410 5.1. One-dimensional advection with constant-velocity

This part employs the equal-limiter scheme for the advection of moments in spatially mono-dimensional problems with the disperse particle size as the only internal coordinate of the PBE. The first example deals with the pure advection of the moments without any source term, while the next examples includes the aggregation/breakage source terms in the moment transport equations. The results are compared with those obtained via a 1<sup>st</sup>-order scheme and the realizable high-order scheme (or quasi-2<sup>nd</sup>-order scheme) by
Vikas et al. [6]. In addition, the analytical solution is reported whenever it
is available.

All the cases use 3-node quadrature to approximate the NDF. This num 420 ber of nodes requires to track the first 6 moments with respect to the par-421 ticle size,  $M^0, M^1, \dots, M^5$ . The calculation of the weights and abscissas of 422 the quadrature is done by using the Chebyshev algorithm. The spatial prob-423 lems are defined over the spatial domain [0, 1], which is discretized to cells 424 of identical size  $\Delta x = 0.01$ . The fluxes at the faces are calculated using 425 high-resolution limited-flux methods. The limiters, in turn, are computed 426 using the minmod function, as it was also used by Vikas et al [6]. Two ghost 427 cells at the left side of the domain and one ghost cell at the right side are 428 considered to cope with the three-cell stencil required by the high-resolution 429 schemes. The advection velocity, u, is set to 1.0 and  $\Delta t$  is calculated by 430 fixing the CFL condition equal to 0.5. The following solution procedure is 431 used to advance in time starting from the initial data, which is based on the 432 explicit fractional-step method for time integration: 433

1. Initialize the moments in the interior domain.

435 2. Apply the boundary conditions at the two left ghost cells.

- 436 3. Calculate the limiters for all the moments at each face.
- 437 4. Find the minimum limiter at each face.
- 438 5. Calculate the flux of the moments using the minimum limiter at each439 face.

- 6. Compute the intermediate values of the moments at each interior cell using the fluxes at the corresponding left and right faces after a time step equal to  $\Delta t$ .
- Find the weights and the abscissas of the quadrature at each interior
  cell using the intermediate values of the moments.
- 8. Calculate the source contributions at each interior cell using the corresponding quadrature approximation of the NDF.
- 9. Advance the intermediate values of the moments at each interior cell by one time step  $\Delta t$  using the calculated source terms.
- 449 10. Apply the boundary condition at the right ghost cell using zero-order
  450 extrapolation from the last interior cell of the domain.

<sup>451</sup> 11. Repeat steps 3 to 10 until obtaining the solution at the desired time.

Steps 8 and 9 (fractional step) approach) are obviously required only if the 452 source terms are present. In this work, the source terms are treated by a 453 single-stage method as explained in steps 8 and 9. However, these steps can 454 be modified to use a two-stage method, leading to higher accuracy for the 455 fractional-step approach as explained by LeVeque [15]. It should be empha-456 sized that this suggestion concerns the application of two-stage methods only 457 for updating the intermediate moments by the source terms. Therefore, no 458 realizability issue is generally expected in case of using two-stage methods 459 instead of one-stage method only to treat the source terms, provided that 460 the intermediate moments after the advection are realizable. Furthermore, 461

step 7 is done even in the case without source term to check the realizabilityof the moments.

464 More details on the problem settings are presented for each case sepa-465 rately.

### 466 5.1.1. Pure advection of the moments

The first example is the one-dimensional pure advection of the moments, i.e. no source term, with the following initial and boundary conditions:

$$IC: \quad M^{k}(x_{i}, 0) = \overset{\circ}{M^{k}} \quad \text{for} \quad i = 0, 1, 2, ..., p$$
$$BC \text{ (ghost cells)}: \quad \begin{cases} M^{k}(x_{-1}, t_{n}) = M^{k}(x_{-2}, t_{n}) = M^{k}_{b} \\ M^{k}(x_{p+1}, t_{n}) = M^{k}(x_{p}, t_{n}) \end{cases}$$
(51)

where the interior cells are numbered from 0 to p. The initial conditions 469  $\overset{\circ}{M^k}$  and the boundary conditions  $M^k_b$  are two sets of scaled moments having 470 the shape of different log-normal distributions,  $\overset{\circ}{Y}$  and  $Y_b$ . The parameters 471 of the distributions, i.e. the mean and the standard deviation of the cor-472 responding normal distributions, are respectively  $(\mathring{\mu}, \mathring{\sigma}) = (\ln(0.008), 0.22)$ 473 and  $(\mu_b, \sigma_b) = (h(0.005), 0.2)$ . Furthermore, the zero-order moments are 474  $\overset{\circ}{M^0} = 20000$  and  $M_b^0 = 800000$  respectively. It should be noted that the two 475 log-normal distributions have different parameters to avoid their quadra-476 ture approximations having the same abscissas. Otherwise, the interpolated 477 abscissas on the faces are identical to those of the cells regardless of the 478 employed scheme. Then, it is trivial to show that, in this special case, the 479 quasi- $2^{nd}$ -order scheme proposed by Vikas et al. [6] is essentially the same 480 as applying 2<sup>nd</sup>-order scheme directly to the moments. 481



Figure 2 compares the results obtained from 1<sup>st</sup>-order scheme, quasi-2<sup>nd</sup>-

order scheme and the proposed equal-limiter scheme. Furthermore, the an-483 alytical solution is plotted in Fig. 2 to provide a benchmark. It is pointless 484 to report the results by the standard 2<sup>nd</sup>-order TVD scheme since, as proved 485 before, the corresponding results would be identical to those obtained by 486 the equal-limiter scheme. As expected, the solution given by the 1<sup>st</sup> order 487 scheme is very diffusive. The quasi-2<sup>nd</sup>-order scheme improves the accuracy 488 of the results by applying 2<sup>nd</sup>-order scheme to the weights. However, the 489 moments do not remain bounded simply because applying a TVD scheme 490 to the weights does not guarantee the boundedness of the transported mo-491 ments, hence appearance of the non-physical oscillations in the solutions. 492 The least oscillations belong to the moment of order zero as expected, since 493 it is simply equivalent to the sum of the weights, the variable to which the 494 TVD scheme is applied in the quasi-2<sup>nd</sup>-order scheme. The oscillations be-495 come more obvious as the moment order increases. It should be noted that, 496 according to our tests, the oscillations may increase or vanish depending on 497 the characteristics of the underlying NDFs. The best predictions belong to 498 the equal-limiter scheme which is indeed the full 2<sup>nd</sup>-order TVD scheme since 490 this numerical example is the same as the pure advection Riemann problem 500 studied in Section 3. Consequently, the predictions are bounded and without 501 any oscillation. 502

## 503 5.1.2. Moment advection with source term

The next examples deal with a more practical application. The moments of a particle size distribution are introduced and advected in the domain while they are subject to local changes due the effect of the aggregation/breakage of the particles. The initial and boundary conditions are the same as the case of pure advection (see Eq. (51)). In the following, two cases are presented in which the aggregation and breakage are considered separately. Both aggregation and breakage are modeled by assuming a constant kernel. For the case of breakage, the daughter size distribution is expressed by assuming symmetric fragmentation of the particles [23]. The reasoning behind these simplistic assumptions is the possibility of obtaining analytical solutions for the moments of the NDF.

<sup>515</sup> Constant aggregation kernel. In this case, the source term in Eq. (7) is <sup>516</sup> calculated as follows [23]:

$$h_{i}^{k} = \frac{1}{2} \sum_{\alpha=1}^{3} w_{i,\alpha} \sum_{\beta=1}^{3} w_{i,\beta} (L_{i,\alpha}^{3} + L_{i,\beta}^{3})^{k/3} K_{a} \sum_{\alpha=1}^{3} L_{i,\alpha}^{k} w_{i,\alpha} \sum_{\beta=1}^{3} w_{i,\beta} K_{a}$$
(52)

517 where  $K_a = 10^{-5} \ (m^3 \cdot s^{-1})$  is the aggregation kernel.

The solutions obtained by the studied schemes are shown in Fig. 3. As can 518 be seen, both quasi-2<sup>nd</sup>-order and equal-limiter schemes improve the accuracy 519 of the results with respect to the 1<sup>st</sup>-order scheme. It is notable that, despite 520 employing the minimum limiter, the equal-limiter scheme produces almost 521 comparable results to those of the quasi-2<sup>nd</sup>-order scheme. Moreover, the 522 solutions of  $M^3$  indicate that only 1<sup>st</sup>-order and equal-limiter schemes are 523 bounded, as expected. Instead, a slight degree of overshoot and undershoot 524 exists in the solution of the quasi-2<sup>nd</sup>-order scheme. The appearance of these 525 spurious oscillations is certainly due to the numerics as both aggregation and 526 breakage of the particles have no effect on the moment of order three with 527 respect to the particle size. Although no analytical solution is available for 528  $M^5$ , some degree of overshoot and undershoot can be observed visually in 529 the solution obtained by the quasi-2<sup>nd</sup>-order scheme. Again it can be seen 530

that the amplitude of the oscillations are intensified as the moment order 531 increases. It is worth mentioning that employing the standard 2<sup>nd</sup>-order 532 TVD scheme is not feasible because the moments get corrupted shortly after 533 starting the simulation and consequently the Chebyshev algorithm fails to 534 calculate the weights and the abscissas required for the source calculation. 535 Even reducing the time step by a factor of 100, equivalent to an impractically 536 small CFL value of 0.005, cannot remedy the non-realizability problem. This 537 shows the effectiveness of the proposed equal-limiter scheme in preserving the 538 realizability of the moments when the 2<sup>nd</sup>-order TVD schemes are employed. 539 Symmetric constant breakage kernel. In this case, the source term in 540 Eq. (7) is calculated as follows [23]: 541

$$h_{i}^{k} = \sum_{\alpha=1}^{3} w_{i,\alpha} 2^{(3-k)/3} L_{i,\alpha}^{k} K_{b} - \sum_{\alpha=1}^{3} w_{i,\alpha} L_{i,\alpha}^{k} K_{b}$$
(53)

<sup>542</sup> where  $K_b = 4$  (s<sup>-1</sup>) is the breakage kernel.

Fig. 4 depicts the results provided by the studied schemes along with the analytical solutions. The same arguments presented for the case of pure aggregation apply also to this case with the difference that here the oscillating behavior of the quasi 2<sup>nd</sup>-order scheme is more intense. This further highlights the advantage of the equal-limiter scheme whenever the boundedness of the solution is strictly required.

## 549 5.2. Pure advection in two-dimensional transient flow

<sup>550</sup> The previous part presents satisfactory results obtained by the equal-<sup>551</sup> limiter scheme in the one-dimensional constant-velocity Riemann problem <sup>552</sup> examples. However, it is important to examine the predictions obtainable <sup>553</sup> by the proposed scheme in systems with higher dimensions and realistic flow

fields, e.g. non-constant and/or transient velocity. For this purpose, a famil-554 iar two-dimensional transient flow, known as lid-driven cavity, is selected to 555 compare the results for the pure advection of moments obtained by employ-556 ing upwind, quasi-2<sup>nd</sup>-order and equal-limiter schemes. The moments belong 557 to the distributions that represent the population of micro-droplets which 558 are transported by a carrier liquid. The micro-droplets are assumed to do 559 not have their own inertia and therefore they move with the same velocity 560 of the carrier liquid. 561

The simulation domain is a square with length (L) of 10 cm and it is dis-562 cretized by a structured uniform Cartesian grid comprising of 10000 square 563 cells of size 1 mm. The flow is confined by four boundaries of type wall, from 564 which the top one moves with the velocity (U) of 1 (m/s) while the others are 565 fixed. The kinematic viscosity of the liquid ( $\nu$ ) is set to  $2.5 \times 10^{-4}$  (m<sup>2</sup>/s), 566 which results to Reynolds number of 400 defined by  $UL/\nu$ . The liquid is 567 assumed to be stagnant at time zero and then a transient flow develops in 568 the liquid due to the constant velocity (U) applied at the top wall. 560

The transient simulations are done by using the icoFoam solver of Open-570 FOAM software, which solves the governing (constant-density) Navier-Stokes 571 equations for the figuid phase numerically by using the PISO algorithm [16]. 572 The time step is set to 0.0001 (s) to keep the maximum Courant number 573 below 0.1. The solution of the velocity field at three time instants are shown 574 in Fig. 5. The solver is modified to solve simultaneously the moment trans-575 port equations. At the beginning of each time step, the moments of the 576 micro-droplet population are advected in time using the velocity field of the 577 previous time step. Then, the flow field of the liquid phase is updated by us-578

ing the PISO algorithm. Regarding the advection of moments, as mentioned 579 in Section 4, the implicit Euler time-integration can be used with the advec-580 tion schemes that deal with the moments directly, and therefore is adopted 581 here when the upwind and equal-limiter schemes are employed. On the other 582 hand, the quasi-2<sup>nd</sup>-order scheme is implemented with Euler explicit time-583 integration. It should be noted that the reasoning behind employing the 584 implicit time-integration scheme is to highlight the advantage of the equal-585 limiter scheme, which is its compatibility with the implicit approach. Con-586 cerning the flux-limiter, the minmod function is used for the interpolation 587 of quadrature weights in case of employing quasi 2nd order scheme and the 588 interpolation of moments in case of employing equal-limiter scheme. 589

Two different cases corresponding to two different initial conditions for the 590 moments are considered. The first initial condition is defined such that there 591 is no micro-droplets in the domain except for a square patch where a popu-592 lation of micro droplets with average size of 100 ( $\mu$ m) and standard devia-593 tion of 20 ( $\mu$ m) is introduced. The population is assumed to be distributed 594 log-normally on the size space. The initial conditions for the moments are 595 calculated based on this log-normal distribution which is scaled to adjust the 596 volume fraction of the micro-droplets equal to 0.05 (assuming spherical shape 597 for the micro-droplets). Fig. 6 depicts the initial conditions for the moment 598 of order three, along with the solutions for the same moment at t = 3 s ob-590 tained by employing the 1<sup>st</sup>-order upwind, quasi-2<sup>nd</sup>-order and equal-limiter 600 schemes. As can be seen, the solution obtained by the upwind scheme suffers 601 from high numerical diffusion. On the other hand, both the quasi-2<sup>nd</sup>-order 602 and equal-limiter schemes yield comparable results, which have higher resolu-603

tion with respect to the one obtained by the upwind scheme. It is noteworthy
that the same contour plots (but of different values) are obtained for the other
moments, which is expected since the shape of the distribution corresponding
to the underlying NDF remains the same in pure advection. As a result, the
abscissas of the quadrature approximation are the same in all the cells of the
domain.

As mentioned previously, the quasi-2<sup>nd</sup>-order scheme interpolates the quadra-610 ture abscissas with a 1<sup>st</sup>-order scheme, whereas it interpolates the quadrature 611 weights with a 2<sup>nd</sup>-order scheme. Therefore, when the quadrature abscissas 612 are the same throughout the domain, the entire resolution of the quasi-2<sup>nd</sup>-613 order scheme for the pure advection of moments is the same as the 2<sup>nd</sup>-order 614 scheme. The reason is that, in this case, the value of abscissas on the faces are 615 the same as those at the cell centers regardless of the employed scheme. Con-616 sequently, the pure advection of moments by interpolating the weights onto 617 the faces with a given 2<sup>nd</sup>-order scheme and then constructing the moments 618 on the faces (using the same abscissas) is equivalent to the pure advection 610 of moments by interpolating the moments directly onto the faces using that 620 2<sup>nd</sup>-order scheme. However, this equivalency is not generally valid when the 621 abscissas are not the same through the domain. Thus, it is worth examining 622 the performance of the schemes in case of existing two different distributions, 623 i.e. having different quadrature abscissas, in the system at time zero. For 624 this purpose, the same square patch (with the same population of micro-625 droplets) defined by the initial conditions of the previous case is considered 626 also here. However, it is assumed that another population of micro-droplet 627 exists outside the square patch, instead of assuming no micro-droplet existing 628

in that zone. Let the population of micro-droplets out of the square patch 629 be also distributed log-normally on the size space with average size equal to 630 50 ( $\mu$ m) and standard deviation of 7.5 ( $\mu$ m). This distribution is scaled to 631 have the volume fraction of the micro-droplets equal to 0.001. Then, the interval 632 tial condition of the moments is defined based on this scaled distribution, as 633 shown in Figs. 7 and 8 for the moments of order zero and three respectively. 634 Moreover, the predictions at t = 3 s are depicted by these figures for the 635 mentioned moments. As can be seen in Fig. 7, the values of  $M_0$  obtained by 636 employing the quasi-2<sup>nd</sup>-order scheme do not remain bounded between the 637 limits defined by the initial conditions. It is noteworthy that in QBMM, the 638 transported variables are indeed the moments and therefore in the pure ad-639 vection with a solenoidal velocity field, the solution for the moments should 640 remain bounded between the limits defined by the initial conditions. This 641 issue concerning the quasi-2<sup>nd</sup>-order scheme can be associated to the fact 642 that this scheme interpolates the weights and abscissas of the quadrature 643 separately, and therefore there is no guarantee that the TVD criteria [20] are 644 respected by this scheme. On the other hand, the solution obtained by the 645 equal-limiter scheme (when it is used with the minimum limiter) respects 646 the boundedness property of the moments. Moreover, the applied change in 647 the initial condition of the moments should not change the pattern of the 648 solution contour plots, since the current initial condition with the two dis-649 tributions can be changed to a problem with initial condition similar to the 650 previous case (micro droplets existing only in a square patches) by a change 651 of variables. However, the comparison between the results shown in Fig. 8 652 with those depicted in Fig. 6 highlights that only the equal-limiter scheme 653

reproduces the same pattern for  $M_3$  in both cases. Furthermore, the pattern of the results obtained by the equal-limiter scheme for  $M_0$  and  $M_3$  shown in Figs. 7 and 8 are the same, whereas this is not the case for the results obtained by the quasi-2<sup>nd</sup>-order scheme. This final example emphasizes the advantage of employing a scheme which interpolates the moments directly, e.g. equal-limiter scheme, instead of interpolating some variables related to the moments.

#### 661 6. Conclusions

A new technique called equal-limiter scheme was proposed to overcome 662 the non-realizability problem that arises when the 2<sup>nd</sup>-order TVD schemes 663 are employed to solve the moment transport equations in the context of 664 QBMM. The central idea behind the technique is that the interpolated mo-665 ments on the faces must form a realizable set when the moment fluxes are 666 being calculated. Following this idea, it was explained that using an identical 667 flux-limiter for all the moments at each face guarantees the realizability of 668 the interpolated moments and consequently helps to preserve the realizabil-669 ity of the transported moments. Although no formal proof has been given 670 to ensure that the equal-limiter scheme preserves the realizability of the mo-671 ments under general conditions, it has been shown that this feature can be 672 achieved in the limit of small time steps (as long as the moment sets are 673 far from the boundary of the moment space). On the contrary, adjusting 674 the time step can not mitigate the non-realizability problem if the limiters 675 are independently calculated for each moment of the transported moment 676 set. This fact was also illustrated by the numerical tests as the moments 677

did not remain realizable even with impractically small time step in the case 678 of employing the standard 2<sup>nd</sup>-order TVD scheme. Moreover, it was proved 679 that the minimum limiter is a possible practical option for the equal limiter 680 if the boundedness feature of the TVD schemes has to be retained. 681 though selecting the minimum limiter may imply solutions of lower order. 682 the one-dimensional numerical examples showed that the results obtained by 683 equal-limiter and quasi-2<sup>nd</sup>-order schemes are comparable in terms of accu-684 racy. More importantly, the improvement in the accuracy was observed also 685 for the solutions obtained by the equal-limiter scheme in a one-way coupled 686 QMOM-CFD simulation of a transient two-dimensional flow. Furthermore, 687 the new technique does not only improve the accuracy of the solution with 688 respect to the 1<sup>st</sup>-order solution but also keeps the solution bounded, which 689 was shown to be an advantage over the quasi-2<sup>nd</sup>-order scheme by comparing 690 their predictions in both one- and two-dimensional numerical examples. In 691 addition, the implementation of the scheme is simple and can be integrated 692 into the CFD simulations easily. 693

The future works will focus on applying the proposed scheme to the three-dimensional CED simulation of polydisperse systems and studying its predictions in comparison to those of the other discretization schemes.

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Figure 1: Flux-limiter functions. The shaded area specifies the TVD region and the hatched area is the 2<sup>nd</sup>-order region by Sweby [21]. The minmod [17] and van Leer [18] limiter functions are shown by the continuous and dashed curves respectively.



Figure 2: Comparison of the results obtained by employing different schemes for the case of pure advection: 1) analytical solution (dot-dashed line); 2) upwind scheme (continuous line); 3) quasi 2<sup>nd</sup>-order scheme (dotted line); 4) equal-limiter scheme (dashed line)



Figure 3: Comparison of the results obtained by employing different schemes for the case of constant aggregation kernel: 1) analytical solution if available (dot-dashed line); 2) upwind scheme (continuous line); 3) quasi 2<sup>nd</sup>-order scheme (dotted line); 4) equal-limiter scheme (dashed line)



Figure 4: Comparison of the results obtained by employing different schemes for the case of symmetric constant breakage kernel: 1) analytical solution (dot-dashed line); 2) upwind scheme (continuous line); 3) quasi 2<sup>nd</sup>-order scheme (dotted line); 4) equal-limiter scheme (dashed line)



Figure 5: Velocity field (m/s) of the simulated 2-D lid-driven cavity flow at three time instants.



Figure 6: Comparison of the studied schemes for the advection of  $M_3$  in the 2-D cavity flow. (a) The initial condition at t = 0; (b) the predictions obtained by employing the different schemes at t = 3.



Figure 7: Comparison of the studied schemes for the advection of  $M_0$  in the 2-D cavity flow in case of existing two different distributions in the domain. (a) The initial condition at t = 0; (b) the predictions obtained by employing the different schemes at t = 3.



Figure 8: comparison of the studied schemes for the advection of  $M_3$  in the 2-D cavity flow in case of existing two different distributions in the domain. (a) The initial condition at t = 0; (b) the predictions obtained by employing the different schemes at t = 3.