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Numerical calculation of the moments of the population balance equation

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Abstract

The combined CFD–PBM (population balance models) are computationally intensive, so a possibility is to calculate only a few moments of the probability density function (PDF) of the PBM minimizing the computational costs. However, this formulation results in an excess of unknowns with respect to equations which is referred to as a closure problem. One approach for dealing with this closure problem is to apply a numerical quadrature approximation. On the other hand, a different possibility is to compute the PDF and from this, the moments of interest if required.

In this work, the two mentioned approaches are discussed and numerical experiments are used to show the capability of the methods for predicting the moments of the PBE. In particular, the quadrature method of moments and a time–space least squares spectral method will be discussed.

Keywords: Population balance equation; Least squares method; Quadrature approximation

1. Introduction

Population balance equations (PBEs) are encountered in several scientific and engineering disciplines, which model complex processes where the accurate prediction of the dispersed phase play major role for the overall behavior of the system. Some examples of this type of processes can be found in systems such as precipitation, crystallization, aerosol, bubbly, droplet flows, and so on. The PBE allows us to describe the dispersed phase by means of a probability density function (PDF) or more general a density function (DE), for instance $f(x, \xi, t)$ where x is the spatial vector position, ξ is the property of interest of the dispersed phase, and t the time. Thus, $f(x, \xi, t)\,\mathrm{d}\xi$ can represent for example the average number of particles per unit volume around the point x at time t, with property between ξ and $\xi + \mathrm{d}\xi$. In this last case, $f(x, \xi, t)$ is called a number distribution function (NDF) [19]. The evolution of this PDF must take into account the different processes that control the PDF such as breakage, coalescence, growth and convective transport of the particles. The result is a nonlinear partial integro-differential equation which requires to be solved by a suitable numerical method.

The method of moments is an efficient method to solve the PBE, but it gives no information about the shape of the distribution and it is only applicable to a limited number of problems. For example, Frenklach [14] applied the method

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of moments to a coagulation process where the coagulation rate was constant. On the other hand, for an arbitrary coagulation rate function, this formulation results in an excess of unknowns compared to the number of equations which is denoted as a closure problem [19]. One way to avoid this problem is to assume the shape of the PDF. Thereby the parameters of the PDF are related closing of the set of moments equations [36]. A second alternative is to express the PDF as a truncated series of some orthogonal polynomials [19]. This approach can be considered a variation of the method of moments in the mathematical framework of the method of weighted residuals (MoM-MWR) [13]. In this case, the test functions are chosen to be power polynomial. The MoM-MWR can be useful in the particular case that the number of moments used is quite small (2 or 3), or exact rational arithmetic is used for example using symbolic manipulation programs like Mathematica or Maple. Otherwise, it is suggested to adopt the eigenfunctions of a singular Sturm–Liouville problem, such as the Chebyshev or Legendre polynomials, for the test functions [4]. However, a lot of effort is being made during the last decade for applying the MoM-MWR for solving the PBE in some particular fields of research, even with its ill-condition property [4].

McGraw [28] proposed a modification of the moment of moments which consists in using a quadrature approximation in order to avoid the closure problem, in problems describing the evolution of aerosols. McGraw [28] based his method on the product difference (PD) algorithm suggested by Gordon [18], calling this approach quadrature method of moments (QMOM). Marchisio et al. [24,26] followed the previous approach to study particulate systems. However, the PD algorithm is a numerical ill-conditioned method for computing the Gauss quadrature rule (e.g. [22]). In general the computation of the quadrature rule based on the power moments of the PDF is quite sensitive to small errors as the number of moments used becomes large (e.g. [17,16]). The applicability of QMOM is limited in general to no more than 12 or 14 moments depending on the problem, although in certain applications it is stated that few moments are enough for obtaining reliable results [29]). Later, McGraw and Wright [30] proposed a new moment closure method, the Jacobian matrix transformation (JMT) which avoids the use of the PD algorithm. Similarly, Marchisio et al. [25] extended the QMOM method to multifluid applications calling this approach the direct quadrature method of moments (DQMOM).

A different way of avoiding the closure problem is discussed in [15] in the method of moments with interpolative closure (MOMIC). In this case, the natural logarithmic of the moments is expressed by a polynomial in the moment order, and thus, the required moments are interpolated or extrapolated. Further discussion about the closure for the method of moments can be found in Diemer and Olson [9]. In this work, we will concentrate only in the QMOM approach.

An alternative approach for computing the moments of the PDF is performed in two stages. First the evolution of the PDF is calculated, then the moments are computed from the PDF. Several methods have been proposed for the latter approach as reviewed by Ramkrishna [34]. However, in order to introduce the population balance framework in computationally demanding environments such as in the simulation of bubble column reactors, high order methods might be a convenient option. In this respect, it is possible to find several examples of the application of high order methods for solving the PBE. For instance, Subramain and Ramkrishna [35] presented a Tau method for solving the distribution of the population of microbial cells that present growth and breakage processes. Mantzaris et al. [24] discuss the Galerkin, Tau and pseudo-spectral methods as a tool for solving multi-variable cell population balance models that present growth and breakage. Chen et al., [5] develop a wavelet-Galerkin method for solving PBEs for the treatment of particle-size distribution in problems of a continuous, mixed-suspension and mixed-product removal crystallizer with effects of breakage. Liu and Cameron [23] proposed the use of a wavelet-based method for the treatment of problems involving particle nucleation, growth and agglomeration.

Recently, Dorao and Jakobsen [10,11] did show the applicability of the least squares method [21,3,33,31] using Legendre polynomials for the particle space discretization and Crank–Nicolson for the time discretization. Later, Dorao and Jakobsen [12] discussed the space–time least squares formulation for solving the PBE. In this space–time formulation time is treated as an additional dimension, which allows high order accuracy both in space and in time (e.g. [7,32]). Thus, space–time can be solved at once, or per time-step on a space–time slab in a kind of semi-discrete formulation.

The motivation for our work is to study two different alternatives for computing the moments evolution of the PDF of linear partial integro-differential equations that occurs in the modeling of breakage type phenomena. The capability of the QMOM and the least squares method for solving such a problem are analyzed studying the effects of some particular breakage functions in the solution accuracy. It is noticed that the QMOM is included in this analysis due to the increasing interest in this method in several engineering research areas, even with its ill-conditioned nature.

In Section 2, the PBE for the breakage case is presented. Section 3 describes the two different numerical methods. In Section 4, some numerical examples are discussed. Finally, Section 5 presents the main conclusions of this work.

2. The population balance equation: pure breakage

The PBE describes the evolution of a density function which represents the collective behavior of a population of particles such as bubbles, droplets or solid particles. For a general discussion, we define the density function $f(\xi, t)$ of a given population with ξ a property of the population e.g., the particle volume, and t the time. The breakage equation without considering spatial dependencies looks like

$$\frac{\partial f(\xi, t)}{\partial t} + \mathscr{L}_b f(\xi, t) = g(\xi, t) \quad \text{in } \Omega = [\xi_{\min}, \xi_{\max}] \times [0, T], \tag{1}$$

$$f(\xi, t) = f_0(\xi) \quad \text{on } \Gamma_0 \tag{2}$$

with $g(\xi, t)$ a source or sink of particles, and

$$\mathscr{L}_b = b(\xi) f(\xi, t) - \int_{\xi_{\min}}^{\xi_{\max}} b(\xi) h(\xi, s) f(s, t)\, \mathrm{d}s \tag{3}$$

the breakage operator. The first term in the RHS of (3) represents the change in the population due to loss of the individuals in the population, for example due to a breakage process; in this case $b(\xi)$ is the *breakage rate* of the particles of type ξ. The second term in the RHS gives us the change in the population due to the arrivals of new individuals with property ξ. In the case of a breakage process, the breakage of particles of type s will produce particles of type ξ according to the *breakage yield function*, $h(\xi, s)$. Besides, $h(\xi, s)$ satisfies the property that

$$h_k(s) = \int_{\xi_{\min}}^{\xi_{\max}} \xi^k h(\xi, s)\, \mathrm{d}\xi = s^k, \tag{4}$$

where $h_k(s)$ is the moment of the new particles that appear after the breakage, if k is the moment that is conserved in the breakage process. For example, assuming that ξ represents the volume of the particle: if the sum of the volume of the particles that appear due to the breakage of a particle with volume s is conserved, then we have that $k = 1$, i.e., the 1th moment is conserved.

Finally, Eq. (2) is the required initial condition, which is applied on $\Gamma_0 = \{(\xi, t) \in \partial\Omega : t = 0\}$.

Some important remarks regarding Eq. (3) can be made. The first one is that Eq. (1) is also known as the *Barbashin Equation* [1]. Furthermore, if the transient term is zero and $b(\xi, t) = 1$, Eq. (3) is called the *Fredholm integral equation of second kind* [6]. The second remark is that in practical application the particle property ξ is restricted by the maximum dimensions of the systems. Thus, we prefer to define the problem directly in the interval $[\xi_{\min}, \xi_{\max}]$ instead of the semi-infinity interval $[\xi_{\min}, \infty)$ usually considered [34]. For simplicity in the notation, in the rest of the paper we will assume that $[\xi_{\min}, \xi_{\max}] \equiv [0, 1]$. The last remark is that the integral term in expression (3) can be expressed like

$$\int_{\xi}^{\xi_{\max}} b(\xi) h(\xi, s) f(s, t)\, \mathrm{d}s \tag{5}$$

assuming that only particle with a property $s > \xi$ can break into ξ. For example this holds when ξ is assumed to be the bubble volume [34]. However, expression (3) is much more general and includes the previous case.

Instead of using Eq. (1) for computing the PDF $f(\xi, t)$ and from this the moments

$$\mu_k(t) = \int_0^1 \xi^k f(\xi, t)\, \mathrm{d}\xi \quad \text{for } k = 0, 1, \ldots. \tag{6}$$

Eq. (1) can be rewritten in a moment form, as shown in the following subsection.

2.1. Moments form of the breakage equation

Eq. (1) and the corresponding initial condition can be transformed to the moment form by multiplying by ξ^k and integrating it. Thus, we get the $2N$ set of equations

$$\frac{\partial \mu_k(t)}{\partial t} + \mathscr{L}_b^k f(\xi, t) = g_k(t), \tag{7}$$

$$\mu_k(0) = \mu_k^0, \tag{8}$$

for $k = 0, 1, \ldots, 2N-1$. The previous enumeration was chosen due to the fact that latter on in QMOM, $2N$ moments equations are required to compute an N points Gauss quadrature rule.

In Eq. (7), each term is defined like

$$\frac{\partial \mu_k(t)}{\partial t} = \int_0^1 \xi^k \frac{\partial f(\xi, t)}{\partial t}\,\mathrm{d}\xi = \frac{\partial}{\partial t}\int_0^1 \xi^k f(\xi, t)\,\mathrm{d}\xi, \tag{9}$$

$$g_k(t) = \int_0^1 \xi^k g(\xi, t)\,\mathrm{d}\xi, \tag{10}$$

$$\mathscr{L}_b^k f(\xi, t) = \int_0^1 \xi^k \mathscr{L}_b f(\xi, t)\,\mathrm{d}\xi, \tag{11}$$

$$= \int_0^1 \xi^k b(\xi) f(\xi, t)\,\mathrm{d}\xi - \int_0^1 \left[\int_0^1 \xi^k h(\xi, s)\,\mathrm{d}\xi\right] b(s) f(s, t)\,\mathrm{d}s, \tag{12}$$

$$= \int_0^1 \xi^k b(\xi) f(\xi, t)\,\mathrm{d}\xi - \int_0^1 h_k(s) b(s) f(s, t)\,\mathrm{d}s. \tag{13}$$

Eq. (7) presents a closure problem due to the excess of the $2N+1$ unknowns ($f(\xi, t)$ and $2N$ moments μ_k) compared with the $2N$ equations. Therefore, one possibility is to express $f(\xi, t)$ in terms of the $2N$ unknowns moments μ_k, in this way the problem can be closed. In the previous section of this paper some methods dealing with this closure problem where mentioned. In the following section, the quadrature approximation of the integral terms based on quadrature rules based on the moments of the PDF will be discussed.

It is important to mention that if K is the moment that is conserved during the breakage, using Eq. (4) we get that $\mathscr{L}_b^K f(\xi, t) = 0$. Therefore, for this pure breakage case, there is at least one moment equation that is closed,

$$\frac{\partial \mu_K}{\partial t} = g_K, \tag{14}$$

$$\mu_K(t) = \mu_0^K. \tag{15}$$

3. Numerical methods

3.1. The quadrature method of moments

The QMOM can be interpreted as a type of the method of moments in the method of weighted residuals (MoM-MWR), although this is not common. Thus, defining the residual function like

$$\mathscr{R}(\xi, t; f) = \frac{\partial f(\xi, t)}{\partial t} + \mathscr{L}_b f(\xi, t) - g(\xi, t) \tag{16}$$

the method of weighted residuals consists in setting the weighted integral of the residual function to zero,

$$\int_0^1 \mathscr{R}(\xi, t; f)\phi\,\mathrm{d}\xi = 0, \tag{17}$$

where ϕ is called the test or weight function. The standard MoM-MWR consists in choosing the test function to be power polynomials, i.e., $\phi_i = \xi^{i-1}$, with $i = 1, \ldots, N$ [13]. While the unknown function f is expressed as a linear combination of the basis functions $\varphi_j(\xi)$,

$$f(\xi, t) = \sum_{j=1}^{N} \alpha_j(t)\varphi_j(\xi), \tag{18}$$

where φ_j are called the trial functions, and α_j are the coefficients of the expansion. Substituting (18) into (17) and after a little of algebra, we get

$$\sum_{j=1}^{N} \frac{\partial \alpha_j(t)}{\partial t}\langle \varphi_j(\xi), \phi_i(\xi)\rangle + \sum_{j=1}^{N} \alpha_j(t)\langle \mathscr{L}_b\varphi_j(\xi), \phi_i(\xi)\rangle = \langle g(\xi, t), \phi_i(\xi)\rangle \tag{19}$$

for $i = 1, \ldots, N$, and where the inner product is defined like

$$\langle \bullet, \bullet\rangle = \int_0^1 \bullet\bullet \, d\xi. \tag{20}$$

Hence, the system of equations given by Eq. (19) dictates the time evolution of the coefficients α_j. Finally, the moments can be computed as

$$\mu_k(t) = \sum_{j=1}^{N} \alpha_j(t)\langle \varphi_j(\xi), \xi^k\rangle. \tag{21}$$

It was mentioned earlier that this approach is considered useful in the particular case in which the number of moments used is relatively small, but in general it is recommended to avoid the use of this framework [4].

The QMOM can be considered as a particular case of the MoM-MWR, where the trial functions, $\varphi_j(\xi)$ are chosen to be Lagrangian interpolant polynomials defined in a non-standard way. These Lagrangian polynomials are defined using the quadrature points given by the quadrature rule constructed using the moments $\mu_i(t)$ of the unknown function $f(\xi, t)$, for example by means of the PD algorithm [18]. Therefore, the time evolution is discretized using an explicit method. The MoM-MWR algorithm equivalent to QMOM can be summarized as:

(1) Given $f(\xi, t)$, the $2N$ moments $\mu_k(t)$ can be computed.
(2) Using the $2N$ moments $\mu_k(t)$ the quadrature rule, $\{\xi_q, w_q\}_{q=1}^{N}$ is obtained by using the PD algorithm.
(3) Using the quadrature points ξ_q the Lagragean interpolant polynomial can be defined. Then, $\phi_j(\xi)$ satisfy the property that $\phi_j(\xi_i) = \delta_{ij}$, if ξ_i is a quadrature point.
(4) The integrals in Eq. (19) are computed using quadrature rule previously obtained, see step 2. For example, considering the first term of the operator $\mathscr{L}_b$ given by expression (3), we have

$$\langle b(\xi)\varphi_j(\xi), \phi_i(\xi)\rangle = \int_0^1 b(\xi)\varphi_j(\xi)\phi_i(\xi)\,\mathrm{d}\xi, \tag{22}$$

$$\approx \sum_{q=1}^{N} \frac{1}{f(\xi_q, t)} b(\xi_q)\varphi_j(\xi_q)\phi_i(\xi_q)w_q, \tag{23}$$

$$\approx \sum_{q=1}^{N} \frac{1}{\alpha_q(t)} b(\xi_q)\delta_{jq}\phi_i(\xi_q)w_q, \tag{24}$$

$$\approx \frac{1}{\alpha_q(t)} b(\xi_j)\phi_i(\xi_j)w_j, \tag{25}$$

where the factor $1/f(\xi, t)$ is introduced in the quadrature approximation, because $f(\xi, t)$ was the measure used for constructing the quadrature rule, and due to the fact that $\varphi_j(\xi)$ are nodal basis functions, $\alpha_q(t) = f(\xi_q, t)$.

(5) Finally, the N coefficients α_j can be predicted at $t + \Delta t$. From this, the moments the $2N$ moments μ_k at $t + \Delta t$ can be approximated like

$$\mu_k(t + \Delta t) \approx \sum_{j=1}^{N} \alpha_j(t + \Delta t)\langle \varphi_j(\xi), \xi^k \rangle. \tag{26}$$

(6) Repeat step 2 until the final time is reached.

In order to be consistent with the standard literature, the most common way of presenting QMOM is also briefly discussed [28,27]. Basically, QMOM consist in avoiding the high order moment dependence by using Gauss quadrature rules. Due to the fact that the density function or the related orthogonal polynomials are not known in order to compute the quadrature rule, the power moments of the density function are used instead, for example using the PD algorithm. Thus, the QMOM approach consists in applying quadrature approximation to the integral terms in $\mathscr{L}_b^k f(\xi, t)$, expression (11),

$$\int_0^1 \xi^k b(\xi, t) f(\xi, t)\, \mathrm{d}\xi = \sum_{q=1}^{N} \xi_q^k b(\xi_q) w_q + \hat{\mathbf{R}}_N^k, \tag{27}$$

$$\int_0^1 h_k(s) b(s) f(s, t)\, \mathrm{d}s = \sum_{q=1}^{N} h_k(\xi_q) b(\xi_q) w_q + \check{\mathbf{R}}_N^k, \tag{28}$$

where the quadrature rule $\{\xi_q, w_q\}_{q=1}^N$ for the interval [0, 1] is computed based on the first $2N$ moments of $f(\xi, t)$.

The terms $\hat{\mathbf{R}}_N^k$ and $\check{\mathbf{R}}_N^k$ are the errors introduced in the approximation of the integral terms. In particular, $\hat{\mathbf{R}}_N^k = 0$ if $(\xi^k b(\xi)) \in \mathbf{P}^{2N-1}([0, 1])$, i.e., a polynomial at most of order $2N-1$. Therefore, for a given value of k=0, 1, …, $2N-1$, the error term $\hat{\mathbf{R}}_N^k = 0$ if $b(\xi) \in \mathbf{P}^{2N-1-k}([0, 1])$, which implies that $\hat{\mathbf{R}}_N^k = 0$ for all k only if $b(\xi)$ is a constant. A similar analysis can be made for $\check{\mathbf{R}}_N^k$.

The final set of equations is

$$\frac{\partial \mu_k(t)}{\partial t} = -\sum_{q=1}^{N} \xi_q^k b(\xi_q) w_q + \sum_{q=1}^{N} h_k(\xi_q) b(\xi_q) w_q + g_k(t) + \mathbf{E}_{\mathrm{QMOM}}^k, \tag{29}$$

$$\mu_k(0) = \mu_k^0, \tag{30}$$

for $k = 0, 1, \ldots, 2N - 1$, where $\mathbf{E}_{\mathrm{QMOM}}^k = \hat{\mathbf{R}}_N^k + \check{\mathbf{R}}_N^k$ is the error introduced by the quadrature approximation.

It is important to note that QMOM is formulated in term of the moments μ_k instead of the coefficients α_j as in the equivalent QMOM derived using the MoM-MWR framework. So, an important drawback of QMOM is that the information needed for constructing the PDF is lost, which is not the case if the equivalent MoM-MWR is used.

It is important to note that if K is the conserved moment after the breakage, then using the conservation statement of Eq. (4), we get

$$\frac{\partial \mu_K(t)}{\partial t} = \underbrace{-\sum_{q=1}^{N} \xi_q^K b(\xi_q) w_q + \sum_{q=1}^{N} \xi_q^K b(\xi_q) w_q}_{=0} + g_K(t), \tag{31}$$

$$\mu_K(0) = \mu_0^K, \tag{32}$$

where the two terms of the breakage process canceled out independent on the functional form of $b(\xi)$ and what it is more important whether the quadrature points and weights $\{\xi_q, w_q\}_{q=1}^N$ are accurate or not. Therefore, at least the evolution of the Kth moment is expected to be correct. This fact will be observed later in the numerical experiments.

The error terms $\mathbf{E}^k_{\mathrm{QMOM}}$ are in part a consequence of neglecting high order terms. In order to understand this fact we can study in a simplified form which are the main contributions to this error term. Simplifying the analysis, we assume that $b(\xi) \in \mathbf{P}^{N_B}([0,1])$. Without loss of generality we further assume that $N_B > 2N+1$ thus the first term of (13) can be expressed like

$$\int_0^1 \xi^k b(\xi,t) f(\xi,t)\,\mathrm{d}\xi = \int_0^1 \xi^k \left[\sum_{i=0}^{N_B} \beta_i \xi^i\right] f(\xi,t)\,\mathrm{d}\xi \tag{33}$$

$$= \sum_{i=0}^{N_B} \beta_i \left[\int_0^1 \xi^{k+i} f(\xi,t)\,\mathrm{d}\xi\right]. \tag{34}$$

Dividing the sum in (34) into two sums such that the first sum contains only polynomials of at most order $2N-1$, and then applying quadrature rules based on the moments of $f(\xi,t)$, we get

$$\sum_{i=0}^{2N-1-k} \beta_i \left[\int_0^1 \xi^{k+i} f(\xi,t)\,\mathrm{d}\xi\right] + \sum_{i=2N-k}^{N_B} \beta_i \left[\int_0^1 \xi^{k+i} f(\xi,t)\,\mathrm{d}\xi\right] \tag{35}$$

$$= \sum_{i=0}^{2N-1-k} \beta_i \left[\sum_{q=1}^{N} \xi_q^{k+i} w_q + \underbrace{\hat{\mathbf{R}}_N^{i,k*}}_{=0}\right] + \underbrace{\sum_{i=2N-k}^{N_B} \left[\beta_i \sum_{q=1}^{N} \xi_q^{k+i} w_q + \underbrace{\beta_i \hat{\mathbf{R}}_N^{i,k}(f)}_{\mathbf{E}^k_{\mathrm{QMOM}}}\right]}_{\mathbf{E}^k_{\mathrm{MOM}}}, \tag{36}$$

where $\hat{\mathbf{R}}_N^{i,k*}(f) = 0$ for all $i = 0,\ldots,2N-1-k$, because the quadrature rule is exact for polynomials of order lower or equal to $2N-1$. On the other hand, $\hat{\mathbf{R}}_N^{i,k}(f) \neq 0$, because the integrand, i.e., ξ^{k+j}, is a polynomial of higher order than $2N-1$. The second term in (36), called $\mathbf{E}^k_{\mathrm{MOM}}$, correspond to the error introduced if the high order moments are explicitly neglected. So, the error $\mathbf{E}^k_{\mathrm{QMOM}}$ is expected to be lower than the one produced if high order moments are explicitly neglected.

3.2. The least squares method

The least squares method (LSQ) is a well established numerical method for solving a wide range of mathematical problems, (e.g. [21,3,33,31]). The basic idea in the LSQ is to minimize the integral of the square of the residual over the computational domain. In the case when the exact solutions are sufficiently smooth the convergence rate is exponential. For time dependent problems, the space–time formulation, i.e., time is treated as an additional dimension, allows high order accuracy both in space and in time (e.g. [7,32]. In this way, space–time can be solved at once, or per time-step on a space–time slab in a kind of semi-discrete formulation. In particular, the application of LSQ to PBE were previously discussed in [10–12].

The least–squares formulation is based on the minimization of a norm-equivalent functional. This consists in finding the minimizer of the residual in a certain norm. The norm-equivalent functional is given by

$$\mathscr{J}(f; g, f_0) \equiv \tfrac{1}{2}\|\mathscr{L}f - g\|^2_{Y(\Omega)} + \tfrac{1}{2}\|f - f_0\|^2_{Y(\Gamma_0)}$$

with

$$\mathscr{L}f = \frac{\partial f(\xi,t)}{\partial t} + \mathscr{L}_b f(\xi,t) \tag{37}$$

a linear integro-differential operator, and the norms defined like

$$\|\bullet\|^2_{Y(\Omega)} = \langle \bullet, \bullet\rangle_{Y(\Omega)} = \int_\Omega \bullet\bullet\,\mathrm{d}\Omega, \quad \|\bullet\|^2_{Y(\Gamma_0)} = \langle \bullet, \bullet\rangle_{Y(\Gamma_0)} = \int_{\Gamma_0} \bullet\bullet\,\mathrm{d}s. \tag{38}$$

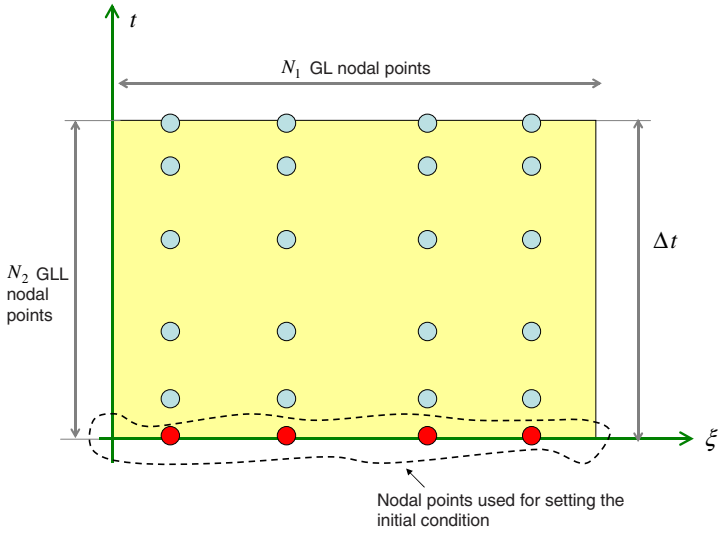

Fig. 1. Nodal points for the LSQ time–space discretization.

Based on variational analysis, the minimization statement is equivalent to:
Find $f \in X(\Omega)$ such that

$$\lim_{\varepsilon \to 0} \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \mathscr{J}(f + \varepsilon v; g, f_0) = 0 \quad \forall v \in X(\Omega), \tag{39}$$

where $X(\Omega)$ is the space of the admissible functions. Consequently, the necessary condition can be written as:
Find $f \in X(\Omega)$ such that

$$\mathscr{A}(f, v) = \mathscr{F}(v) \quad \forall v \in X(\Omega) \tag{40}$$

with

$$\mathscr{A}(f, v) = \langle \mathscr{L} f, \mathscr{L} v \rangle_{Y(\Omega)} + \langle f, v \rangle_{Y(\Gamma_0)}, \tag{41}$$

$$\mathscr{F}(v) = \langle g, \mathscr{L} v \rangle_{Y(\Omega)} + \langle f_0, v \rangle_{Y(\Gamma_0)}, \tag{42}$$

where $\mathscr{A} : X \times X \to \mathbb{R}$ is a symmetric, continuous bilinear form, and $\mathscr{F} : X \to \mathbb{R}$ a continuous linear form. The discretization statement consists in searching the solution in a reduced subspace, i.e., $f_N(r, \xi) \in X_N(\Omega) \subset X(\Omega)$. Therefore, f_N can be expressed like

$$f_N(\xi, t) = \sum_{i=0}^{N_1} \sum_{j=0}^{N_2} f_{ij} \varphi_i(\xi) \varphi_j(t) \tag{43}$$

$$= \sum_{l=0}^{\mathscr{N}} f_l \Phi_l(\xi, t) \quad \text{with } f_l = f_{ij} = f(\xi_i, t_j), \tag{44}$$

where $\Phi_l(\xi, t) = \varphi_i(\xi)\varphi_j(t)$ with $l = i + j(N_1+1)$ and $\mathscr{N} = (N_1+1)(N_2+1)-1$. The 2D basis functions Φ_l are expressed like the products of 1D basis functions $\varphi_i(\xi)$ and $\varphi_j(t)$. In particular, in this work $\varphi_i(\xi)$ and $\varphi_j(t)$ are chosen to be the 1D Lagrangean interpolants through the Gauss–Legendre (GL) collocation points and Gauss–Lobatto–Legendre (GLL) collocation points, respectively [8]. The total number of nodal points f_l, which are the number of unknowns to be determined is referred to as the number of degrees of freedom $N_{\mathrm{dof}} = (N_1 + 1)(N_2 + 1)$. Fig. 1 shows an example of the distribution of the nodal points.

Replacing approximation (43) into Eq. (40), and choosing systematically $v = \Phi_0, \ldots, \Phi_{\mathcal{N}}$, we get the final algebraic system

$$\mathscr{A}\boldsymbol{f} = \mathscr{F}, \tag{45}$$

where

$$[\mathscr{A}]_{ij} = \mathscr{A}(\Phi_j, \Phi_i) = \langle \mathscr{L}\Phi_j, \mathscr{L}\Phi_i \rangle_{Y(\Omega)} + \langle \mathscr{B}\Phi_j, \mathscr{B}\Phi_i \rangle_{Y(\Gamma_0)}, \tag{46}$$

$$[\mathscr{F}]_i = \mathscr{F}(\Phi_i) = \langle g, \mathscr{L}\Phi_i \rangle_{Y(\Omega)} + \langle f_0, \mathscr{B}\Phi_i \rangle_{Y(\Gamma_0)}, \tag{47}$$

$$[\boldsymbol{f}]_i = f_i = f(x_i). \tag{48}$$

After solving one time slab (Δt), the procedure is repeated until reaching the final simulation time T.

Finally, the moments evolution can be computed using expression (6).

4. Numerical experiments

Although, it is possible to find some analytical cases for the homogeneous breakage problem, i.e., $g(\xi, t) = 0$ [37], for studying the effects of the polynomial order in the error term of QMOM the inhomogeneous form of the problem is used. The model problem is not directly related to any particular system, the breakage rate function $b(\xi)$ was chosen with different complexities in order to study the effects of this function in the quadrature approximation. Actually, the breakage rate and redistribution functions commonly used in the modeling of some processes such as bubble column reactors involves complex functional dependencies (e.g. [20]). The suggested problem is given like

$$\frac{\partial f(\xi, t)}{\partial t} = -b(\xi) f(\xi, t) + \int_0^1 b(\xi) h(\xi, s) f(s, t)\, \mathrm{d}s + g(\xi, t), \tag{49}$$

$$f(\xi, 0) = f_0(\xi), \tag{50}$$

where $\xi \in [0, 1]$, and where the analytical solution, except for case 1D for which no analytical solution is available, is given by

$$f(\xi, t) = 2 - e^{-t},$$

$$f_0(\xi) = 1.$$

The considered subcases are defined as

$$\text{A} \quad b(\xi) = \xi^2, \quad g(\xi, t) = e^{-t} + (-2 + e^{-t})\left(\tfrac{4}{3} - \xi^2\right), \tag{51}$$

$$\text{B} \quad b(\xi) = \xi^6, \quad g(\xi, t) = e^{-t} + (-2 + e^{-t})\left(\tfrac{16}{5} - \xi^4\right), \tag{52}$$

$$\text{C} \quad b(\xi) = 2\xi^9 e^{-\xi^2}, \quad g(\xi, t) = e^{-t} - 2(2 - e^{-t})\left(12 - \frac{65}{2e}\right) + 2\xi^9 e^{-\xi^2}(2 - e^{-t}), \tag{53}$$

$$\text{D} \quad b(\xi) = 2\xi^9 e^{-\xi^2}, \quad g(\xi, t) = 0, \tag{54}$$

with $h(\xi, s) = 1$ for all the subcases, so the breakage process conserves the 0th moment.

In the following discussion, the normalized moments $\overline{\mu}_k(t)$ are used, which are given as

$$\overline{\mu}_k(t) = \frac{\mu_k(t)}{\mu_k(0)}. \tag{55}$$

In order to show how good the numerical solutions of the above problems are in comparison with the exact ones, we shall use the weighted 1-norm $\|\varepsilon_k(t)\|_1$ defined by

$$\|\varepsilon_k(t)\|_1 = \left| \frac{\mu_k(t) - \mu_{k,N}(t)}{\mu_k(t)} \right|, \tag{56}$$

where $\mu_k(t)$ and $\mu_{k,N}(t)$ are the exact and numerical moments, respectively. The maximum error in the simulation $\|\varepsilon_k\|_\infty$ is defined as

$$\|\varepsilon_k\|_\infty = \max_{t\in(0,T)} (\|\varepsilon_k(t)\|_1). \tag{57}$$

The two methods are implemented in Matlab. In particular, the time integration of QMOM is based on an Explicit Runge Kutta 4th order (ERK4) method with a fix time stepping. In order to reduce the source of errors, $g_k(\xi, t)$ and $h_k(s)$ are given explicitly. In the plots referring to QMOM, $2N$ is the number of moments equations.

The LSQ approach is based on the time–space least squares method using different approximation orders for the particle property (N_1) and for the time (N_2). Besides fixed time slabs are used. The integration of the terms involved in Eq. (45) is performed using numerical quadrature based on the same quadrature points as employed for the Lagrangean polynomials. Due to the fact that the output of LSQ is the density function $f(\xi, t)$, the time evolution of the error in the computation of the density function measured in the L^2-norm

$$\|\varepsilon(t)\|_2 = \left(\int_0^1 (f(\xi, t) - f_N(\xi, t))^2 \,\mathrm{d}\xi\right)^{1/2} \tag{58}$$

is computed, where $f(\xi, t)$ is the exact solution and $f_N(\xi, t)$ is the LSQ solution. Besides, the error and residual over the total time–space domain Ω are also computed measured in the L^2-norm

$$\|\varepsilon\|_2 = \left(\int_0^T \int_0^1 (f(\xi, t) - f_N(\xi, t))^2 \,\mathrm{d}\xi \,\mathrm{d}t\right)^{1/2}, \tag{59}$$

$$\|R\|_2 = (\|\mathscr{L} f_N - g\|^2_{Y(\Omega)} + \|f_N - f_0\|^2_{Y(\Gamma_0)})^{1/2}. \tag{60}$$

4.1. Numerical results

For the particular case of $b(\xi) = 1$ and $h(\xi, s) = 1$ which is not included in the test cases, the QMOM solution is excellent because this problem does not present a closure problem, not being necessary to use the QMOM approach.

Fig. 2 shows the evolution of the normalized moments $\overline{\mu}_k(t)$ and the corresponding error $\|\varepsilon_k(t)\|_1$ obtained by QMOM for case 1A and 1B using $2N = 4$ moments equations and $\Delta t = 0.1$. In Fig. 2, the evolution of all the normalized moments computed with the exact solution overlap in one line, and they all coincide with the QMOM solution for the 0th moment that is well computed. Note that for the case 1A the percentual error, i.e., $100\|\varepsilon_k(t)\|_1$, in the computation of the moments is around 5%, except for the 0th moment where $\|\varepsilon_k(t)\|_1$ is around 10^{-7}. For the case 1B the percentual errors increase reaching a 20% error. As it can be seen, the higher the polynomial order of $b(\xi)$, the bigger the error introduced. This can be considered rather obvious for this type of methods based on the projection concept. However, the results presented in this paper show that the common assumption that only a few moments, normally 2 or 4, can be sufficient for obtaining an accurate solution should be carefully reconsidered. Besides, the number of moments required are strongly dependent on the characteristics of the kernel functions.

The results can be improved by increasing the number of moments used, as will be shown later. However, the number of moments used cannot exceed 12 or 14 moments, because of the ill-conditioned nature of the method for computing the quadrature rule.

In Fig. 3, the graph on the left shows the behavior of $\|\varepsilon(t)\|_2$ for the LSQ computation of $f(\xi, t)$ for case 1A, for a time stepping $\Delta t = 1$. In this case, a polynomial of degree $N_1 = 3$ for the particle property and $N_2 = 3$ for the time, i.e., $N_{\mathrm{dof}} = (N_1 + 1)(N_2 + 1) = 16$ is used. The error in the computation of the moments from $f(\xi, t)$ is presented on the right graph in Fig. 3. In this case, N_1 can be lower considering that the PDF is uniform. The time evolution is well resolved inclusive using a Δt equal to the fastest characteristic time of the breakage process, i.e.,

$$\tau_{\min} = \min_{\xi\in[0,1]} \frac{1}{b(\xi)}. \tag{61}$$

In the following, QMOM and LSQ are compared considering error convergence and time computation. In particular, the computational time or wall time, t_{wall}, should be considered as a rough estimate, since no particular optimization was performed for the solvers.

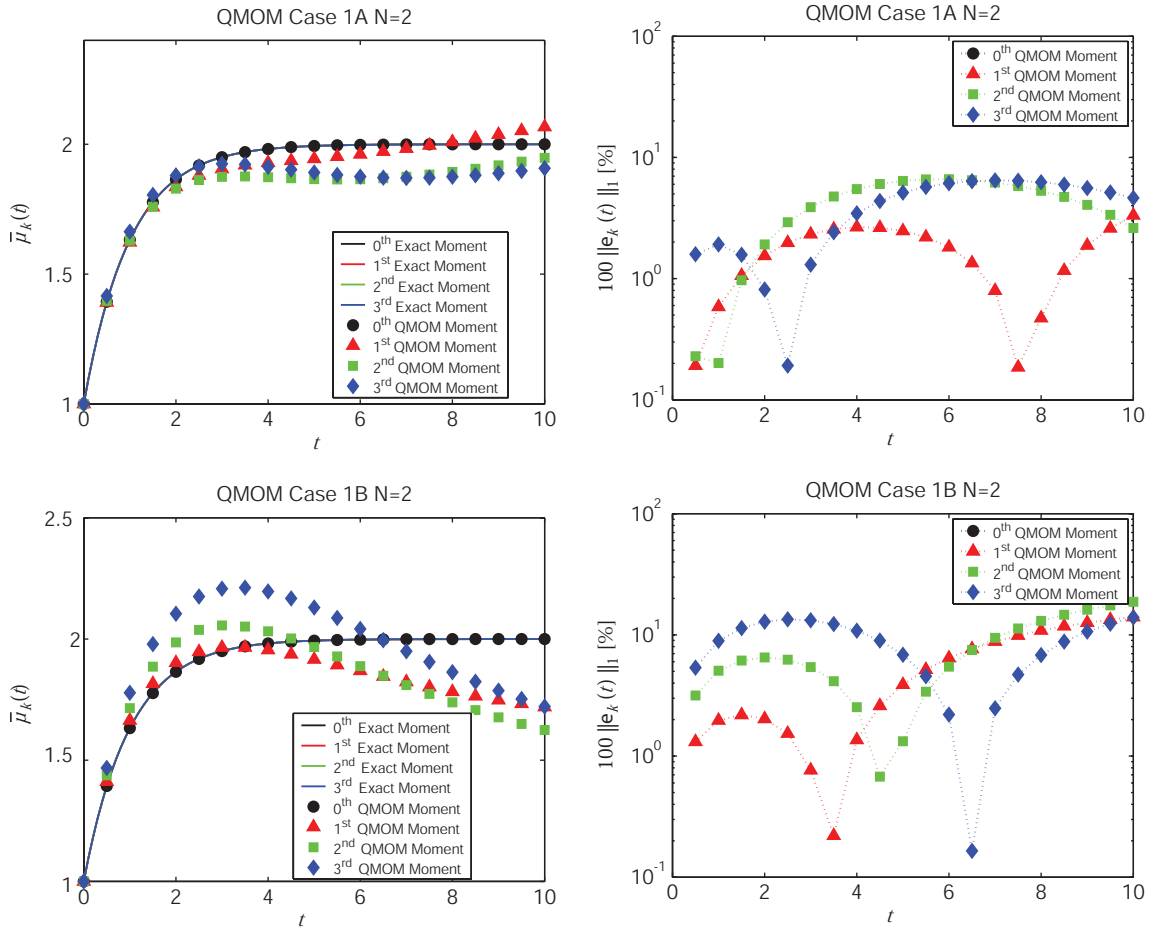

Fig. 2. Moments evolution for case 1A ($b(\xi) = \xi^2$) and case 1B ($b(\xi) = \xi^6$) using QMOM, $\Delta t = 0.1$. Note that the evolution of all the normalized moments computed with the exact solution overlap in single line which coincide with the QMOM solution of the 0th moment.

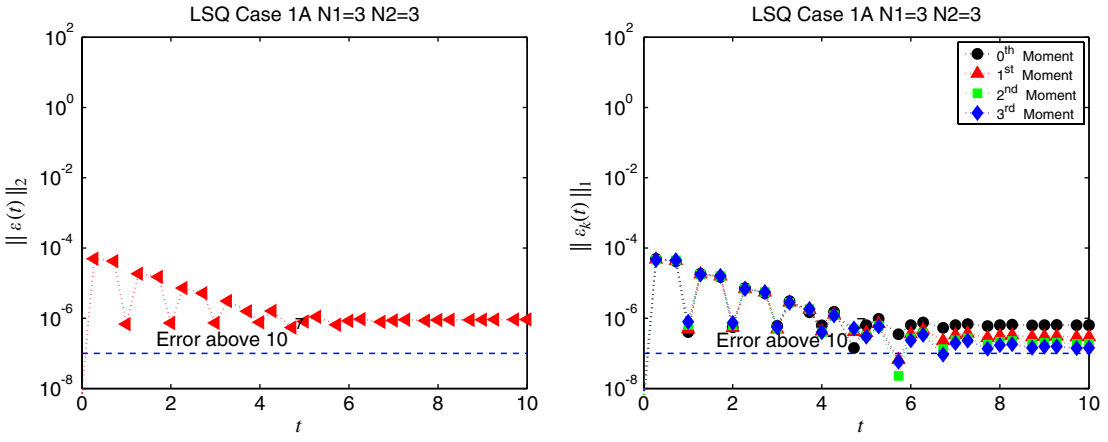

Fig. 3. Behavior of the $\|\varepsilon(t)\|_2$ and $\varepsilon_k(t)$ for case 1A using LSQ ($\Delta t = 1$), $\|R\|_2 = 3.18 \cdot 10^{-3}$, $\|\varepsilon\|_2 = 4.50 \cdot 10^{-5}$.

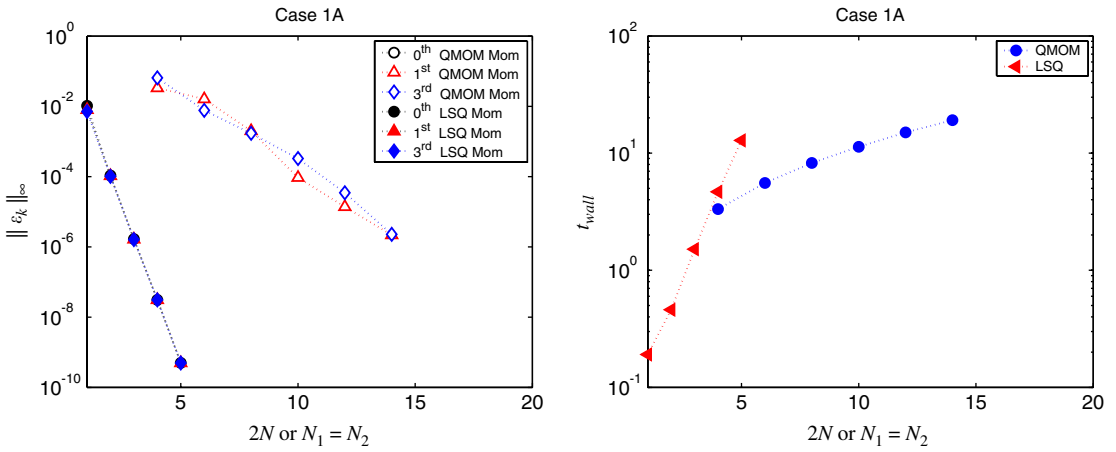

Fig. 4. Error convergence and time computation for case 1A using QMOM ($2N$) and LSQ ($N_1 = N_2$).

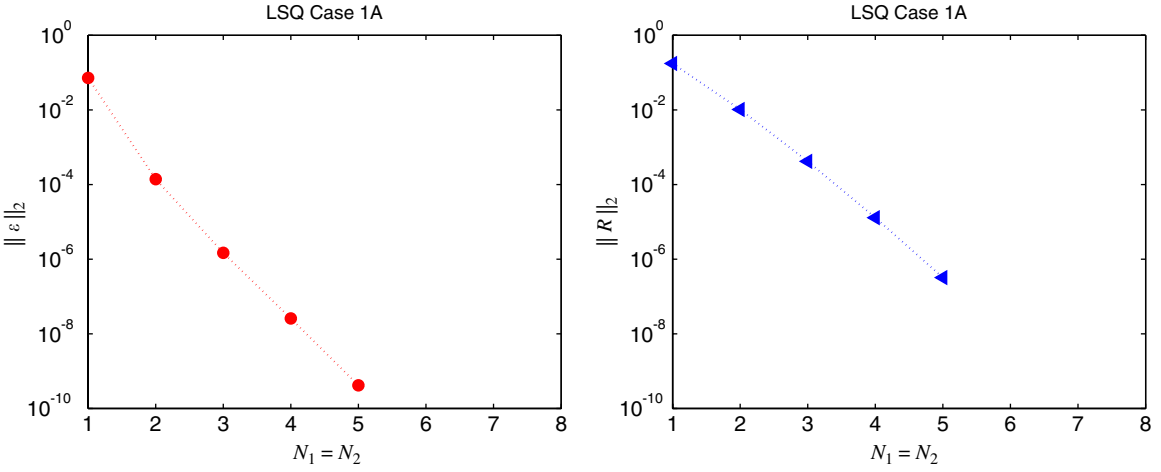

Fig. 5. Error and residual convergence in the L_2-norm for case 1A.

The error convergence rate and computation time of QMOM and LSQ for case 1A are plotted in Fig. 4. In the case of QMOM the time stepping is $\Delta t = 0.01$, which is enough in order to the time integration became the dominant error. In the case of LSQ the time stepping is $\Delta t = 0.5$ and the approximation order in time and space were both varied simultaneously, i.e., $N_1 = N_2$. Due to the different characteristics of the methods, it is quite difficult to compared both methods in a fair way. Both of them show exponential convergence rate. As for QMOM, the convergence rate is a consequence of improving the quadrature rule as the number of moments considered ($2N$) increases. On the other hand, the convergence rate for LSQ is due to the improvement in the time approximation (N_2) in this case. For this case, given a certain value of $N_1 = N_2$, LSQ shows a lower $\|\varepsilon_k\|_\infty$ compared with QMOM with the equivalent $2N$ moments and at the same time a lower computational time t_{wall}. Finally, in Fig. 5 the behavior of $\|\varepsilon\|_2$ and $\|R\|_2$ in the computation of $f(\xi, t)$ using LSQ is shown for the same case 1A.

A similar analysis can be made for case 1B and 1C. The error convergence rates are presented in Fig. 6. The time stepping using QMOM is $\Delta t = 0.01$, while for the case of LSQ it is $\Delta t = 0.5$ and both approximation orders are varied simultaneously, i.e., $N_1 = N_2$.

In the following, case 1D is presented for which the analytical solution is not available. Fig. 7 shows the evolution of $f(\xi, t)$ using LSQ with $N_1 = 5$, $N_2 = 2$ and $\Delta t = 0.5$ and $\|R\|_2 = 5.88 \cdot 10^{-4}$. Considering that the LSQ solution is acceptable, we want to compare the moments prediction using QMOM, see Fig. 8. In this case the time stepping for

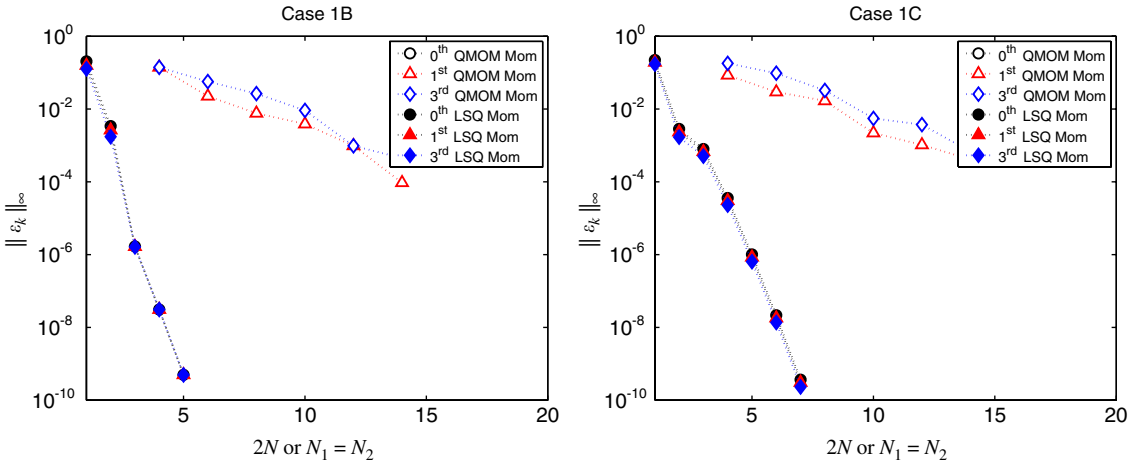

Fig. 6. Error convergence for case 1B and 1C using QMOM ($2N$) and LSQ ($N_1 = N_2$).

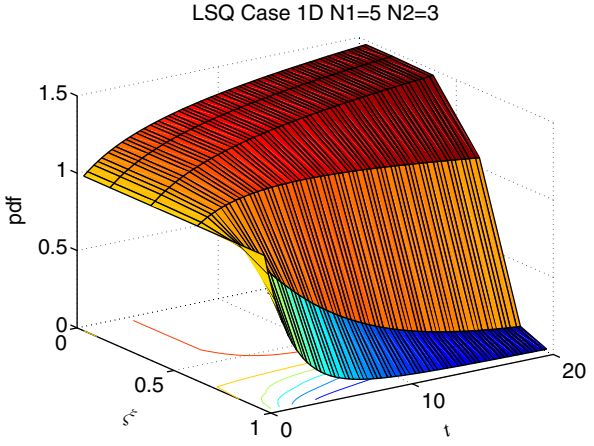

Fig. 7. Evolution of $f(\xi, t)$ for the case 1D using LSQ, $\|R\|_2 = 5.88 \cdot 10^{-4}$ and $\Delta t = 0.2$.

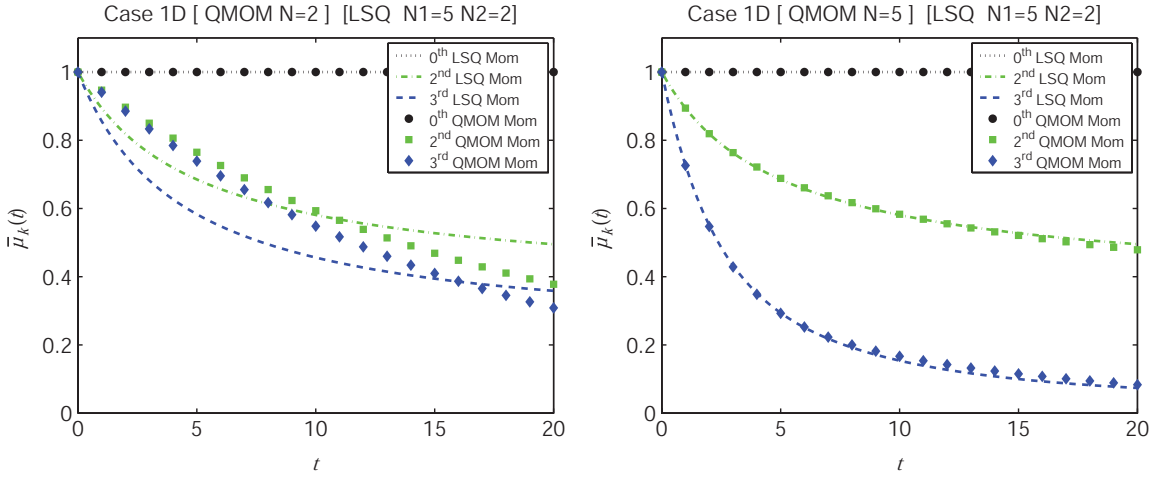

Fig. 8. Comparison in the moments evolution for case 1D using QMOM and LSQ.

QMOM is $\Delta t = 0.05$. Using only $2N = 4$ moments the error in the prediction is higher than 10%, but by increasing the number of moments, for example for $2N = 10$ moments, the error can be reduced. In particular, for $2N = 12$ moments both solutions coincide. It is important to note that for this particular case it was necessary to use the maximum number of moments (12 for this case) in order for the QMOM and LSQ solutions to coincide. This fact can be considered an important drawback of QMOM for more general problems due to the limited capability of analyzing the convergence of the solution.

Finally, it is noticed that in the presented cases the density function evolves to a steady state. Thus, the dynamic behavior of the moments was not studied in details. On the other hand, in most of the practical applications of the PBE, the evolution of the density function is a continuous dynamic process. Nevertheless, in this work it was shown that the high order moments are not well represented using QMOM, and that the higher the order of the moment, the higher the error in the prediction, see Fig. 2. Due to the fact that the QMOM is based on a quadrature rule which is computed using the moments of the density function, it can be expected that the error of the higher order moments will pollute the prediction of the low order moments too. In Fig. 2 the effect mentioned is observed noting that the percentual error in the low order moments increases with time. However, more work is required for studying the pollution effects. The results of such studies will determine the applicability and/or limitation of the QMOM in the simulation of dynamics processes related to specific industrial applications. For the case of LSQ no such pollution effects are observed, so that the error in the moments become more tight, as seen in Fig. 3. The loss of accuracy for LSQ, as for all the projection methods, is a consequence of the nature of the underline solution. Nevertheless, LSQ presents an optimal least-squares a posteriori error estimator [2] which can be used for assessing the quality of computations.

5. Conclusions

The problem of computing the moments of the PBE was studied. In particular, due to its importance for CFD–PBM codes, the moment form of the PBE was particularly discussed because it is usually assumed that this can minimize the computational costs. The moment formulation results in an excess of unknowns with respect to equations which is referred to as a closure problem. One approach for dealing with this problem is to apply the QMOM approach which consists in using a numerical quadrature approximation. A different possibility is to compute the density function and from this, the moments of interest. This can for example be performed using the LSQ method.

It was found that both methods, QMOM and LSQ, are able to predict the moment evolution fairly well for the numerical problem proposed. The nature of the kernel functions determine the number of moments that should be used in the case of QMOM for reaching a certain accuracy. The higher the polynomial order of the kernel functions, the higher the number of moments required for getting reliable predictions. This fact can reduce the applicability of QMOM for example in the simulation of bubbly flows where the kernels functions can have quite complex functional dependence. However, QMOM can be still be used in some applications where the kernels functions are given as a low order polynomials like in some particle or crystallization problems. If the density function is also required the MoM-MWR framework could be used instead for QMOM. In general, more work is required for understanding the consequences of using the QMOM compared with the MoM-MWR.

LSQ shows to be computational efficient and accurate for the tested problem. Besides, computing the moments from the density function using LSQ can be much faster and more accurate compared to QMOM. LSQ provides also information about the reliability of the solution in the residual, which can be used for controlling the time stepping in an efficient way.

Further investigation is required for studying the impact on the accuracy using $\mathscr{C}^0$ functions for the kernels in the QMOM approach. These functions are representative for some practical applications. In this case, the convergence rate of quadrature approximation can be affected.

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