Chemical Engineering Science 176 (2018) 306–318

Contents lists available at ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

# An open-source quadrature-based population balance solver for OpenFOAM

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## HIGHLIGHTS

- Implemented extended quadrature method of moments into OpenFOAM.
- Robust algorithm ensuring moment realizability.
- Verification and validation in 0-D aggregation and breakup problems.
- Validation for aggregation and breakup problem in Taylor-Couette reactor.

## ARTICLE INFO

*Article history:*
Received 13 July 2017
Received in revised form 25 October 2017
Accepted 26 October 2017
Available online 27 October 2017

*Keywords:*
Extended quadrature method of moments
Log-normal kernel density function
Population balance equation
Aggregation and breakage
OpenFOAM
OpenQBMM

## ABSTRACT

The extended quadrature method of moments (EQMOM) for the solution of population balance equations (PBE) is implemented in the open-source computational fluid dynamic (CFD) toolbox OpenFOAM as part of the OpenQBMM project. The moment inversion procedure was designed (Nguyen et al., 2016) to maximize the number of conserved moments in the transported moment set. The algorithm is implemented in a general structure to allow the addition of other kernel density functions defined on $\mathbb{R}^+$, and arbitrary kernels to describe physical phenomena involved in the evolution of the number density function. The implementation is verified with a set of zero-dimensional cases involving aggregation and breakage problems. Comparison to the rigorous solution of the PBE provides validation for these cases. The coupling of the EQMOM procedure with a CFD solver to address aggregation and breakage problems of non-inertial particles is validated against experimental measurements in a Taylor-Couette reactor from the literature.


## 1. Introduction

The spatial and temporal evolution of a discrete population of particles can be described by a population balance equation (PBE) (Ramkrishna, 2000), which is an evolution equation for the number density function (NDF) associated to the particle population. The NDF can evolve due to discontinuous phenomena such as nucleation, aggregation, breakage and evaporation, and due to continuous phenomena such as convection and diffusion. Examples of industrial processes, involving the evolution of a particle population include, but certainly are not limited to, precipitation, polymerization and combustion (Becker et al., 2014), sprays (Laurent and Massot, 2001) and aerosols (McGraw, 1997; McGraw and Wright, 2003).

In this work, we concentrate on the case of a NDF with only one internal coordinate, representing the particle size. Approximate solutions of the corresponding PBE can be determined using several approaches, including Monte-Carlo methods (Lin et al., 2002; Meimaroglou and Kiparissides, 2007; Rosner and Yu, 2001; Smith and Matsoukas, 1998; Zhao et al., 2007; Zhao and Zheng, 2013), which, however, present challenges in practical applications due to their computational cost. Some authors introduce a discretization along the size variable, leading to the sectional method or the method of classes (Alopaeus et al., 2006; Balakin et al., 2014; Bannari et al., 2008; Becker et al., 2011; Hounslow et al., 1988; Hounslow, 1990; Kumar and Ramkrishna, 1996a,b; Muhr et al., 1996; Puel et al., 2003; Vanni, 2000). Similarly to Monte Carlo methods, this approach is often computationally too demanding when applied to large-scale problems of industrial interest, as observed by Marchisio et al. (2003b). To overcome this issue, hybrid methods between sectional and moment methods are developed

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https://doi.org/10.1016/j.ces.2017.10.043
0009-2509/

(see Nguyen et al. (2016) and references therein), but they are not the subject of this paper.

A widely adopted and sufficiently accurate approach to find approximate solutions of the PBE for engineering applications is the quadrature method of moments (QMOM), originally introduced by McGraw (1997), and extensively applied to several problems in chemical engineering (see Gavi et al. (2007), Marchisio and Fox (2013), Petitti et al. (2010) for examples). The QMOM approach considers a discrete set of moments of the NDF, constituted by an even number of moments. The NDF is then approximated with a discrete weighted sum of Dirac delta functions, uniquely determined by means of a moment inversion algorithm (Gautschi, 2004; Gordon, 1968; Wheeler, 1974). The extended QMOM (EQMOM) (Yuan et al., 2012) introduced the capability of using a basis of non-negative kernel density functions (KDF) to approximate the NDF in place of Dirac delta functions. This development allows some of the limitations of QMOM, that appear when dealing with problems that require the evaluation of the NDF at a particular value of the internal coordinate (i.e. problems involving evaporation term or any other continuous size decreasing term (Massot et al., 2010)), to be addressed. Yuan et al. (2012) proposed the EQMOM procedure for $\beta$ and $\Gamma$ KDF, while Madadi-Kandjani and Passalacqua (2015) considered log-normal KDF. The EQMOM reconstruction can be done for every realizable moment set (i.e. moments of a positive NDF), just not reproducing, eventually, the last moment. In particular, it can deal with the degenerate cases, encountered when the moments are not strictly realizable: the only possible representation of the NDF is then a sum of weighted Dirac delta functions, thus describing a population of particles of only one or a few sizes, as in the case of nucleation. Numerically, this possibility was achieved with the moment inversion algorithm of Nguyen et al. (2016).

In this work we discuss the implementation of the EQMOM approach into the open-source toolbox for computational fluid dynamics (CFD) OpenFOAM (2015), as part of the OpenQBMM (2016a) project. We limit our attention to a univariate PBE, where the internal coordinate of the NDF is the particle size. We describe the implementation of EQMOM with log-normal KDF as an example, but without loss of generality in the presentation of the computational framework, which was designed to accommodate any KDF defined on the set of positive real numbers $\mathbb{R}^+$. We then discuss the implementation of realizable kinetic fluxes for advection, which guarantee the transported moments are realizable if the step used for time integration satisfies a realizability condition similar to the Courant-Friedrichs-Lewy condition. Particular attention is put in detailing the implementation of the procedure used to determine the approximate NDF, which always ensures that the maximum possible number of moments is conserved (Nguyen et al., 2016). The PBE solver is then verified considering aggregation and breakage problems studied by Vanni (2000), comparing the predicted results with both the rigorous solution from Vanni (2000) and the numerical solution obtained with EQMOM by Madadi-Kandjani and Passalacqua (2015). Finally, a case involving spatial transport is considered for validation purposes, which consists of an aggregation and breakage problem in a Taylor–Couette reactor. The system was experimentally studied by Serra and Casamitjana (1998a,b), Serra et al. (1997), considering the same test case discussed in Marchisio et al. (2003a). Numerical results obtained with the CFD-PBE solver developed as part of the present work are compared to experiments, showing satisfactory results.

## 2. The population balance equation

The PBE (Marchisio et al., 2003a; Marchisio and Fox, 2013; Ramkrishna, 2000; Randolph and Larson, 1988) accounting for the evolution of a univariate NDF with internal coordinate $\xi$, representing the particle size, is

$$\frac{\partial n(\xi,\mathbf{x},t)}{\partial t}+\nabla_{\mathbf{x}}\cdot[n(\xi,\mathbf{x},t)\mathbf{U}]-\nabla_{\mathbf{x}}\cdot[\Gamma\nabla_{\mathbf{x}}n(\xi,\mathbf{x},t)]+\nabla_{\xi}\cdot[G(\xi)n(\xi,\mathbf{x},t)]$$
$$=\bar{B}^a(\xi,\mathbf{x},t)-\bar{D}^a(\xi,\mathbf{x},t)+\bar{B}^b(\xi,\mathbf{x},t)-\bar{D}^b(\xi,\mathbf{x},t)+\mathcal{N}(\xi,\mathbf{x},t) \quad (1)$$

where $n(\xi,\mathbf{x},t)$ is the NDF, $\mathbf{U}$ is the velocity of the carrier fluid, $\Gamma$ is the diffusivity, $G(\xi)$ is the growth rate, $\bar{B}(\xi,\mathbf{x},t)$ and $\bar{D}(\xi,\mathbf{x},t)$ are, respectively, the rate of change of $n$ due to birth and death, in the aggregation process when the $a$ exponent is present and in the breakage process when a $b$ exponent is present, and $\mathcal{N}(\xi,\mathbf{x},t)$ the rate of change due to nucleation. Let us notice that we assumed the particle size is sufficiently small to have negligible influence on the carrier fluid. This allows the velocity $\mathbf{U}$ to be assumed equal to the local fluid velocity, and independent of the particle size.

The diffusivity $\Gamma$, assumed to be independent from the particle size $\xi$, is defined as the sum of a laminar and a turbulent contribution: $\Gamma=\Gamma_l+\Gamma_t$. The turbulent diffusivity is calculated as the ratio of the turbulent viscosity $\mu_t$ and the turbulent Schmidt number $\sigma_t:\Gamma_t=\mu_t/\sigma_t$.

Following Marchisio and Fox (2013), Marchisio et al. (2003b), Randolph and Larson (1988), the terms describing aggregation and breakage phenomena are written in continuous form as:

$$\bar{B}^a(\xi,\mathbf{x},t)=\frac{\xi^2}{2}\int_0^{\xi}\frac{\beta\left(\left(\xi^3-\xi'^3\right)^{1/3},\xi'\right)}{\left(\xi^3-\xi'^3\right)^{2/3}}n\left(\left(\xi^3-\xi'^3\right)^{1/3},\mathbf{x},t\right)n(\xi',\mathbf{x},t)\mathrm{d}\xi', \quad (2)$$

$$\bar{D}^a(\xi,x,t)=n(\xi,\mathbf{x},t)\int_0^{\infty}\beta(\xi,\xi')n(\xi',\mathbf{x},t)d\xi', \quad (3)$$

$$\bar{B}^b(\xi,\mathbf{x},t)=\int_{\xi}^{\infty}a(\xi')b(\xi|\xi')n(\xi',\mathbf{x},t)\mathrm{d}\xi', \quad (4)$$

$$\bar{D}^b(\xi,\mathbf{x},t)=a(\xi)n(\xi,\mathbf{x},t). \quad (5)$$

Growth and nucleation terms were not considered in the example applications presented in this work to verify and validate the implementation of the EQMOM procedure, however they have been implemented in the PBE solver, and their testing is left to future work. These terms and their numerical approximation in quadrature methods are kept in the description of the theory presented in this work for completeness and as documentation of the code implementation for the interested reader. Their numerical integration is performed in the OpenQBMM framework in an identical manner to that used for the source terms due to aggregation and breakup (Nguyen et al., 2016).

## 3. The extended quadrature method of moments

The approximate solution of the PBE of Eq. (1) is obtained in this work by solving transport equations for a finite set of the moments of the NDF. In the case of a univariate NDF, the moments are defined as:

$$M_k(t)=\int_0^{+\infty}n(\xi,\mathbf{x},t)\xi^k\mathrm{d}\xi. \quad (6)$$

The transport equation for the moment of order $k$ is obtained by multiplying the PBE (Eq. (1)) by $\xi^k$ and integrating over $[0,+\infty[$. Under the previously discussed assumptions on the velocity and the diffusivity, such transport equation is (Marchisio and Fox, 2013; Marchisio et al., 2003b)