



New developments of the Extended Quadrature Method of Moments to solve Population Balance Equations

Maxime Pigou^{a,b,*}, Jérôme Morchain^a, Pascal Fede^b, Marie-Isabelle Penet^c,
Geoffrey Laronze^c

^a LISBP, Université de Toulouse, CNRS, INRA, INSA, Toulouse, France

^b Institut de Mécanique des Fluides de Toulouse – Université de Toulouse, CNRS-INPT-UPS, Toulouse, France

^c Sanofi Chimie – C&BD Biochemistry Vitry - 9 quai Jules Guesde, 94400 Vitry-sur-Seine, France



ARTICLE INFO

Article history:

Received 17 October 2017

Received in revised form 15 February 2018

Accepted 16 March 2018

Available online 21 March 2018

Keywords:

Extended Quadrature Method of Moments (EQMOM)

Quadrature Based Method of Moments (QBMM)

Population Balance

Mathematical modelling

Gauss quadrature

ABSTRACT

Population Balance Models have a wide range of applications in many industrial fields as they allow accounting for heterogeneity among properties which are crucial for some system modelling. They actually describe the evolution of a Number Density Function (NDF) using a Population Balance Equation (PBE). For instance, they are applied to gas–liquid columns or stirred reactors, aerosol technology, crystallisation processes, fine particles or biological systems. There is a significant interest for fast, stable and accurate numerical methods in order to solve for PBEs, a class of such methods actually does not solve directly the NDF but resolves their moments. These methods of moments, and in particular quadrature-based methods of moments, have been successfully applied to a variety of systems. Point-wise values of the NDF are sometimes required but are not directly accessible from the moments. To address these issues, the Extended Quadrature Method of Moments (EQMOM) has been developed in the past few years and approximates the NDF, from its moments, as a convex mixture of Kernel Density Functions (KDFs) of the same parametric family. In the present work EQMOM is further developed on two aspects. The main one is a significant improvement of the core iterative procedure of that method, the corresponding reduction of its computational cost is estimated to range from 60% up to 95%. The second aspect is an extension of EQMOM to two new KDFs used for the approximation, the Weibull and the Laplace kernels. All MATLAB source codes used for this article are provided with this article.

© 2018 Elsevier Inc. All rights reserved.

1. Introduction

Population Balance Equations (PBEs) are particular formalisms that allows describing the evolution of properties among heterogeneous populations. They are used to track the size distribution of fine particles [1]; the bubble size distribution in gas–liquid stirred-tank reactors or bubble columns [2,3]; the crystal-size distribution in crystallizers; the distribution of biological cell properties in bioreactors [4,5]; the volume and/or surface distribution of soot particles in flames [6,7] or the formation of nano-particles [8], among other examples.

* Corresponding author at: LISBP-INSA Toulouse, 135 Avenue de Ranguel, 31077 Toulouse, France.

E-mail address: maxime.pigou@insa-toulouse.fr (M. Pigou).

Nomenclature			
Greek symbols		\mathbf{A}	transition matrix to degenerated moments
ε	relative tolerance	b	orthogonal polynomials recurrence coefficient
λ_j	j -th nested quadrature node	\mathcal{H}	Hankel determinant
μ	positive measure	\mathbf{J}_n	n order Jacobi matrix
ω_j	j -th nested quadrature weight	m_k	moment of order k
Ω_ξ	NDF support	\mathcal{M}	realisable moment space
π_k	k order orthogonal polynomial	n	number density function
σ	shape parameter	\tilde{n}	approximation of n
ξ	random variable	N	order of moment set
ξ_i	i -th main quadrature node	\mathcal{N}	order of realisability
ζ	realisability criteria on $]0, +\infty[$	p_k	canonical moment of order k
Roman		P	number of main quadrature nodes
a	orthogonal polynomials recurrence coefficient	Q	number of nested quadrature nodes
		w_i	i -th main quadrature weight

A PBE describes the evolution and transport of a Number Density Function (NDF), under the influence of multiple processes which modify the tracked property distribution (e.g. erosion, dissolution, aggregation, breakage, coalescence, nucleation, adaptation, etc.).

One often requires low-cost numerical methods to solve PBEs, for instance when coupling with a flow solver (e.g. Computational Fluid Dynamics software). Monte-Carlo methods constitute a stochastic resolution of the population balance and can be applied to such PBE–CFD simulations [9]. Similarly, sectional methods allow direct numerical resolutions of the PBE through the discretisation of the property space [10,11]. They respectively require a high number of parcels or sections in order to reach high accuracy and are thus often discarded for large-scale simulations.

An interesting alternative approach lies in the field of methods of moments. A PBE, which describes the evolution of a NDF, is transformed in a set of equations which describes the evolution of the moments of that distribution. Moments are integral properties of NDFs, the first low order integer moments are related to the mean, variance, skewness and flatness of the statistical distributions described by NDFs. This approach then reduces the number of resolved variables to a finite set of NDF moments. It also comes with some difficulties when one must compute non-moment integral properties, or point-wise evaluations, of the distribution [12].

To tackle these issues, one can try to recover a NDF from a finite set of its moments. In most cases, this reverse problem has an infinite number of solutions and different approaches exist to identify one or an other out of them. The simplest is probably to assume that the NDF is a standard distribution (Gaussian, Log-normal, ...) whose parameters will be deduced from its first few moments. Other methods that lead to continuous approximations, and which preserve a higher number of moments, are the Spline method [13], the Maximum-Entropy approach [12,14,15] or the Kernel Density Element Method (KDEM) [16].

More recently, the Extended Quadrature Method of Moments (EQMOM) was proposed as a new approach which is more stable than the previous ones, and yields either continuous or discrete NDFs depending on the moments [1,17,18]. EQMOM has been implemented in OpenFOAM [19] for the purpose of PBE–CFD coupling. The core of this method relies on an iterative procedure that is a computational bottleneck.

The current work focuses on EQMOM and develops a new core procedure whose computational cost is significantly lower than previous implementations by reducing both (i) the cost of each iteration and (ii) the total number of required iterations.

The previous core procedure [1] will be recalled before describing how it can be shifted toward the new – cheaper – approach. Both implementations will be compared in terms of computational cost (number of required floating-point operations) and run-time.

Multiple variations of EQMOM exist, the Gauss EQMOM [17,20], Log-normal EQMOM [21] as well as Gamma and Beta EQMOM [18]. Two new variations, namely Laplace EQMOM and Weibull EQMOM, are proposed along with a unified formalism among all six variations.

The whole source code used to write this article (figures and data generation) is provided as supplementary data, as well as our implementations of EQMOM in the form of a MATLAB functions library [22].

Download English Version:

<https://daneshyari.com/en/article/6928869>

Download Persian Version:

<https://daneshyari.com/article/6928869>

[Daneshyari.com](https://daneshyari.com)