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Extension of moment projection method to the fragmentation process

Shaohua Wu [a], Edward K.Y. Yapp [b], Jethro Akroyd [b], Sebastian Mosbach [b], Rong Xu [c], Wenming Yang [a], Markus Kraft [b,c,*]

[a] Department of Mechanical Engineering, National University of Singapore, Engineering Block EA, Engineering Drive 1, 117576, Singapore
[b] Department of Chemical Engineering and Biotechnology, University of Cambridge, New Museums Site, Pembroke Street, Cambridge, CB2 3RA, United Kingdom
[c] School of Chemical and Biomedical Engineering, Nanyang Technological University, 62 Nanyang Drive, 637459, Singapore

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ABSTRACT

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

1. Introduction

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

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

* Corresponding author at: Department of Chemical Engineering and Biotechnology, University of Cambridge, New Museums Site, Pembroke Street, Cambridge, CB2 3RA United Kingdom.
E-mail address: mk306@cam.ac.uk (M. Kraft).

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A number of methods have been proposed to solve these types of equations which can be broadly classified as: method of moments (MOM) (see, e.g., Refs. [2,4–7,9–21]), sectional method (see, e.g., Refs. [1,9,22–29]) and stochastic method (see, e.g., Refs. [11,30–35]). These methods often encompass a trade-off between physical detail and computational efficiency. In the stochastic method the particle population is represented by an ensemble of stochastic particles and the particle processes are treated probabilistically [36]. The stochastic solution has been proven to converge to the deterministic solution of the PBE [33]. The method easily allows a highly detailed particle description; however, under certain conditions, the computational time [34] and memory requirement [35] can be intractable. Sectional methods divide the mass range into a finite number of sections [24]. The PSD within each section evolves according to a ordinary differential equation which can be solved by standard solvers (see, e.g., Refs. [25–28]). The computational time rapidly scales with the number of internal coordinates tracked and the number of sections required to achieve convergence [29].

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

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

In Ref. [38] a finite-size domain complete set of trial functions method of moments (FCMOM) is proposed which uses a series of Legendre polynomials to reconstruct the PSD, thus closing the moment equations. However, because only a finite number of polynomials can be determined, certain values of the reconstructed PSD can be negative [39]. An alternative method is the extended quadrature method of moments (EQMOM) where a set of non-negative continuous kernel density functions such as gamma, beta and lognormal functions is adopted to approximate the PSD. In terms of the reconstructed PSD this method can achieve very high accuracy and is able to handle the shrinkage problem. However, information about the shape of the PSD is needed *a priori* to select a suitable kernel density function. Both FCMOM and EQMOM are focused on the reconstruction of the PSD while for most practical applications only the first few moments are needed.

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

For quadrature-based moment methods a very important consideration is the realisability of the moment set [43]. Realisability is related to the existence of an underlying PSD that corresponds to a set of moments. The moments are linked to each other under complex mathematical relationships. If the numerical schemes do not preserve these relationships the set of moments can be unrealisable, i.e., no PSD can be described by such moments or they lead to unphysical distributions (e.g. negative weights and abscissas). The generation of unrealizable moments usually arises from the spatial transportation of moments [44]. Even if a suitable closure is established for the moment transport equation, numerical advection and diffusion schemes can still lead to unrealizable moment sets. This realisability problem can be avoided by properly designing the numerical schemes. For example, recently in Ref. [45] a high-order-volume-schemes for quadrature-based moment methods is introduced to guarantee the realisability of moments. The idea of the discretization scheme is to construct the moment flux terms through interpolation of the quadrature weights rather than the moments at the faces of the cells. By doing this the realisability problem can be prevented. Another scheme developed to preserve the realisability of moments can be found in Ref. [46] where the moments are not transported directly. Instead they use the canonical moments which are easy to control and guarantee the moment vector to stay in the moment space by transporting them separately. In light of realisability, here we restrict our attention to the moment closure method. The aim is to investigate the MPM error in isolation. Therefore we are simulating a spatially homogeneous PBE with no moment advection and diffusion terms. The moments always remain realizable during the whole simulation time span. While for the application of MPM to spatially inhomogeneous systems, moments realizability can be guaranteed by adopting the realizable finite-volume methods.