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# Solution of population balance equations in applications with fine particles: Mathematical modeling and numerical schemes

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ABSTRACT

The accurate description and robust simulation, at relatively low cost, of global quantities (*e.g.* number density or volume fraction) as well as the size distribution of a population of fine particles in a carrier fluid is still a major challenge for many applications. For this purpose, two types of methods are investigated for solving the population balance equation with aggregation, continuous particle size change (growth and size reduction), and nucleation: the extended quadrature method of moments (EQMOM) based on the work of Yuan et al. [52] and a hybrid method (TSM) between the sectional and moment methods, considering two moments per section based on the work of Laurent et al. [30]. For both methods, the closure employs a continuous reconstruction of the number density function of the particles from its moments, thus allowing evaluation of all the unclosed terms in the moment equations, including the negative flux due to the disappearance of particles. Here, new robust and efficient algorithms are developed for this reconstruction step and two kinds of reconstruction are tested for each method. Moreover, robust and accurate numerical methods are developed, ensuring the realizability of the moments. The robustness is ensured with efficient and tractable algorithms despite the numerous couplings and various algebraic constraints thanks to a tailored overall strategy. EQMOM and TSM are compared to a sectional method for various simple but relevant test cases, showing their ability to describe accurately the fine-particle population with a much lower number of variables. These results demonstrate the efficiency of the modeling and numerical choices, and their potential for the simulation of real-world applications.



## 1. Introduction

The evolution of a population of fine, that is non-inertial, particles in a carrier fluid can be described by a population balance equation (PBE) [1–10]. There are many potential applications such as soot modeling, aerosol technology, nanoparticle synthesis, microbubbles, reactive precipitation, and coal combustion (see [5] and references therein). The PBE is a transport equation for the number density function (NDF) of the particles. The NDF depends on time, spatial location and the internal coordinates, which can include, for example, volume, surface area or chemical composition. The mathematical form

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of a typical PBE includes spatial transport (*e.g.* convection and diffusion), derivative source terms for continuous particle size change (*e.g.* oxidation/dissolution and surface growth), integral terms (*e.g.* aggregation and breakage), and Dirac-delta-function source terms describing the formation of particles (*e.g.* nucleation). Moreover, it is usually not only important to predict the evolution of global quantities of the particle population, but also to have some information on the NDF. For example, when considering soot, the total produced mass or volume fraction, as well as the size-dependent NDF represent essential elements in present and future emission regulations. But since the evolution of the NDF is usually coupled with the resolution of the Navier–Stokes equation for the carrier fluid [10], the cost of its resolution has to be reasonable so that the global simulation will be affordable. We therefore seek a robust method able to describe accurately some global quantities of the particle population, but also able to give a good idea of the shape of the NDF, at a reasonable cost.

In this work, only size is considered as the internal variable. Moreover, even if the geometry of fine particles can be complex, we assume that only one variable, *e.g.* volume $v$, is needed to describe it, eventually taking into account the more complex shape of large particles compared to smaller ones through a fractal dimension depending on size. This work thus represents a first step before considering more complex models that add another internal coordinate variable. Different methods are available in the literature to solve the PBE. The Monte-Carlo method [2] is usually too costly to be coupled with a flow solver, especially when considering particle interactions like aggregation. We therefore focus on deterministic methods.

With one internal variable, deterministic methods can be based on a discretization along the size variable. Equations are written for the total number density or the total mass density of the particles inside each interval of the size-discretization. These intervals are called sections in what follows, in reference to the sectional methods, which fall in this category. A large literature is devoted to this type of method, especially for the resolution of the aggregation and/or breakage PBE (see *e.g.* [11–13] and references therein). Among them are the fixed-pivot [11] and the cell-average [14] techniques, which consider that the particle population of one section is represented by only one size (pivot size), the new particles after collision or breakup being distributed over the sections in such a way that the discrete equations are consistent with the global number and mass (they are said to be "moment preserving"), or also with higher order moments [15]. These methods have been generalized to growth, nucleation and aggregation [16,17]. Some other methods are based on a "conservative form" of the PBE for the mass density function [18,19]: a conservative finite-volume method developed for aggregation and breakup [18,19] and extended to growth and nucleation [20], or some moment-preserving methods [21]. These methods have been shown to be convergent when considering only aggregation or breakup, with first-order accuracy for the finite-volume methods [18,19] and second-order accuracy for the fixed-pivot and cell-average techniques [22–24]. But a large number of sections is always used and the ability of these methods to describe adequately the NDF with a small number of sections has not been fully explored, especially for the complete problem with nucleation and growth. Moreover, to our knowledge, such methods have never been reported for cases where the particle size is decreasing through a continuous process.

A different kind of method, the only one that will be called sectional here (even if some of the previous ones are also called sectional in the literature), is based on a closure through a continuous reconstruction of the NDF inside each section. This reconstruction can be constant [25–27] or affine [28]. When considering sprays, sectional methods are also called "Eulerian multi-fluid methods" [26] or "one–size moment" method (OSM), and they are developed after reduction of the internal variables to only size thanks to velocity moments and a mono-kinetic closure. The corresponding model is a finite-volume method. It was shown to be first-order accurate in the pure-evaporation case [29] and exhibited first-order numerical accuracy for the investigated cases, taking into account the collisions (coalescence) [30]. Moreover, in this approach, an affine reconstruction of MUSCL type was tested in the pure-evaporation case. However, if its order of accuracy is higher, the effective accuracy is not much improved compared to the first-order method, except with a large number of sections. Then, as with other discretized methods, sectional methods lead to an accurate prediction of the NDF with a large enough number of sections. However, for many applications, physical transport must also be considered, as well as coupling with the carrier fluid. This can be done thanks to the use of an operator-splitting method (see *e.g.* [31]), but if a large number of sections has to be considered, the computational cost can be prohibitive, since one has to transport at least one variable per section.

In contrast, moment methods do not use a direct resolution of the NDF, but rather transport a finite set of its moments, usually the first few integer order ones. Since they are the moments of a non-negative NDF (or, more rigorously, a positive measure), this moment set belongs to a space strictly included in $\mathbb{R}_+^N$, where $N$ is the number of moments [32–34]. This space is called the moment space. The NDF cannot be recovered from this finite moment set: there is an infinite number of possibilities in non-degenerate cases, *i.e.* when the moment set is in the interior of moment space, whereas a unique sum of weighted Dirac delta functions is possible for the degenerate cases, *i.e.* for the boundary of moment space. One can remark that the degenerate case can appear in problems of interest due to nucleation of fine particles just as they begin to aggregate. Most importantly, moment methods give access to some important properties of the NDF.

For moment methods, two major issues arise. The first is closure of the moment equations due to the nonlinear source terms in the PBE. This includes the negative flux due to the disappearance of particles when continuous size reduction is considered (*e.g.* oxidation or evaporation), which requires a point-wise evaluation of the NDF [35]. Two kinds of closures are used in the literature: (i) a functional dependence of the unclosed terms (usually expressed through some fractional moments) is provided using the moment set; (ii) a NDF, or its corresponding measure, is reconstructed from the moment set, allowing evaluation of all the unclosed terms. In the first category, one finds the interpolative closure (MOMIC) [36,37] widely used in the soot community and extended to the bivariate case [38]. MOMIC is based on an interpolation along the order of the moments. However, this kind of method does not allow one to deal with the disappearance fluxes, except for the hybrid