Solution of population balance equations in applications with fine particles

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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). There are many potential applications such as soot modeling, aerosol technology, nanoparticle synthesis, microbubbles, reactive precipitation, and coal combustion [1]. 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 are still major challenges. For this purpose, two kinds of methods are investigated for solving the PBE: the extended quadrature method of moments (EQMOM) [2] and a hybrid method (TSM) between the sectional and moment methods, considering two moments per section [3]. For both methods, the closure is based on 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.

The major issue associated with moment methods is realizability: the moments must remain in a convex moment space [4, 5]. This usually leads to unphysical results (*e.g.* invalid moment sets). Even if the closure itself ensures the realizability at the continuous level, the classical schemes for high-order transport in physical space can lead to an invalid moment set [6, 7, 8], as well as for transport in phase space, especially when considering continuous particle size reduction and/or the transition between a Dirac distribution (due to the nucleation) and a smooth distribution (due to the aggregation/coagulation).

We develop robust and accurate numerical methods to ensure the realizability of moments for all physical-chemical phenomena [9] and transport in physical space [10]. Moreover, the robustness is also ensured with efficient and tractable algorithms despite the numerous couplings and various algebraic constraints thanks to a tailored overall strategy. Numerical results demonstrate the efficiency (computational cost) of the modeling and numerical choices, and their potential for the simulation of industrial applications.

Keyword: population balance equation, quadrature-based moment method, EQMOM, sectional method, TSM, realizable scheme, finite volume, kinetic scheme

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