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Implementation of bivariate population balance equations in CFD codes for modelling nanoparticle formation in turbulent flames

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In recent years the problem of studying particle formation and dynamics in turbulent flames has become more and more important, for both environmental and technological reasons. On the one hand, toxicological and environmental studies have focused the attention of the combustion community on the accurate modelling of the formation of carbonaceous nano- and microparticle (soot) in turbulent flames; on the other hand, combustion sintesized nanoparticles are gaining growing importance in a wide range of applications. In both cases, information on size and morphology of the particulate matter is required, since these characteristics largely influence the effects of particles on human health and global climate (in the case of soot), and the features of the produced material (in the case of combustion synthesis). In these cases, the solution of the population balance equation (which is a balance equation in terms of the distribution of one or more particle state variables, or internal coordinates) have to be integrated with fluid-dynamics computation within a CFD code, which needs to be employed for the simulation of temperature, composition and velocity fields of the flame. Among all the possible methods for the solution of the population balance, only moments based methods can be coupled with CFD computation, due to their relatively low computational cost. In particular the recently proposed Direct Quadrature Method of Moments (DQMOM) is a promising approach for the simulation of particle dynamics, allowing the solution of the bivariate population balance equation with low additional computational effort. This is an important issue when an accurate description of the evolution of particle morphology (fractal dimension) is required. The use of a single internal coordinate in fact is not sufficient to obtain complete information on the morphological properties of fractal aggregates, such as those often encountered in combustion formed particulate; only the use of two internal coordinates (e.g., volume and area) allows to describe the evolution of particle morphology without strong assumptions on the fractal dimension of the aggregates.

In this work, the DQMOM is applied to the study of soot formation in turbulent non-premixed flames. The model takes into account nucleation, molecular growth, oxidation and aggregation of particles; simplified kinetic rates are employed, while velocity and scalar fields are computed by RANS simulation based on the k-ε model and on the presumed beta-PDF with equilibrium chemistry for the simulation of turbulence-chemistry interaction. At first the monovariate population balance is solved, and the possibilities of treating particle morphology with only one internal coordinate are explored. The bivariate formulation of the DQMOM is then validated by comparison with a direct simulation Monte Carlo code, and the monovariate formulation (in terms of particle volume) is compared with the bivariate formulation (in terms of particle volume and surface area). Simulation results show that the DQMOM is a suitable tool for the solution of the considered problem both in the monovariate and in the bivariate case, and evidence the importance of a proper treatment of particle fractal dimension to obtain accurate predictions of the morphological properties of soot aggregates.

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