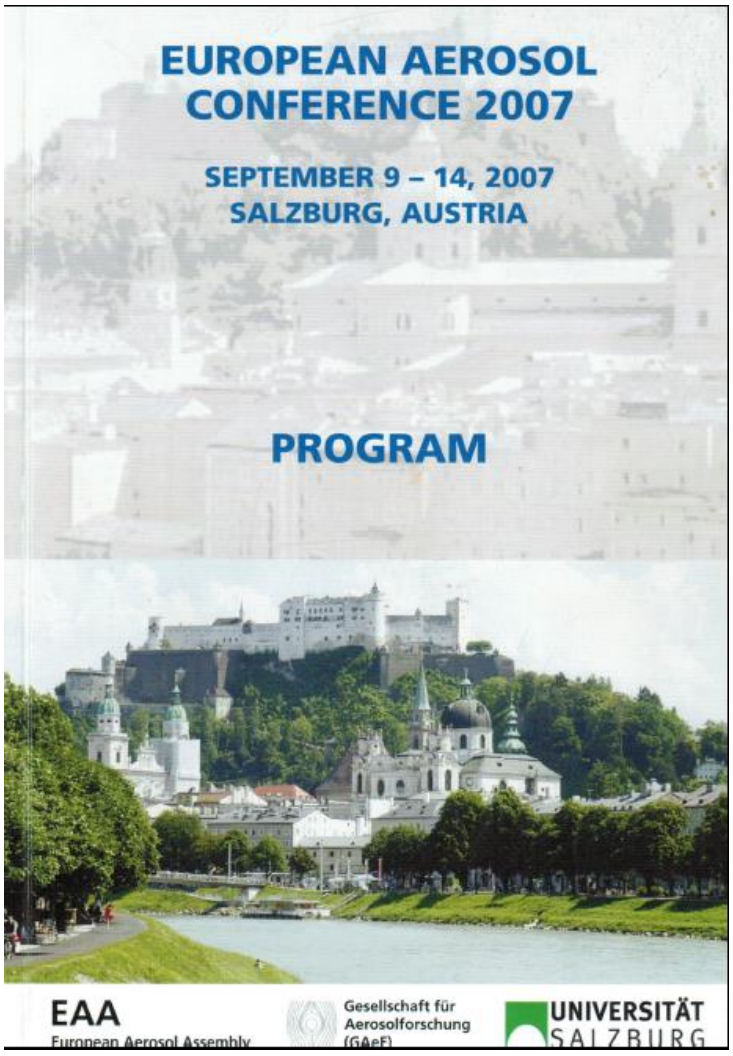


**FORMULATION AND VALIDATION OF MONO- AND BI-VARIATE POPULATION BALANCE MODELS AND THEIR APPLICATION ON SOOT FORMATION IN TURBULENT FLAMES**

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# Formulation and validation of mono- and bi-variate population balance models and their application on soot formation in turbulent flames

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There are a number of applications where it is crucial to simulate the evolution of a particulate system with great accuracy, tracking both the changes in particle structure as well as particle transport phenomena. Particle formation in turbulent flames is a relevant example, notably in the case of soot production in combustion processes (as a by-product) as well as in flame aerosol synthesis reactors.

In order to describe the evolution of these particulate systems, Computational Fluid Dynamics (CFD) is often coupled with a Population Balance Equation (PBE). A very convenient strategy to tackle this problem is the use of the method of moments based on a quadrature approximation. In particular, in this work we focus on the use of Direct Quadrature Method Of Moments, DQMOM (Marchisio and Fox, 2005) for solving mono- and bi-variate PBE, assessing the accuracy of the method by comparison with simulations carried out with Monte Carlo Methods (MCM).

Soot is a by-product of incomplete hydrocarbon combustion and its importance is due to its impact on human health and because of its responsibilities in the climate change. In non-premixed turbulent flames there are a range of complex physical and chemical phenomena involved that strongly and nonlinearly interact.

The evolution of the population of soot particles is written in terms of the Number Density Function (NDF) $\tilde{n}(N;\mathbf{x},t)$, that depends on the number of primary particles per aggregate ($N$), space ($\mathbf{x}$) and time ($t$). The Favre-averaged PBE, omitting spatial and temporal dependencies, results in the following equation:

$$\frac{\partial}{\partial t}\left[\overline{\rho}\tilde{n}(N)\right]+\frac{\partial}{\partial x_i}\left[\overline{\rho}\tilde{U}_i\tilde{n}(N)\right]-\frac{\partial}{\partial x_i}\left[\overline{\rho}(\Gamma+\Gamma_t)\frac{\partial\tilde{n}(N)}{\partial x_j}\right]=\overline{\rho}J(\mathbf{x},t)\delta(N-1)$$
$$+\overline{\rho}\frac{1}{2}\int_0^N\beta(N-N^*,N^*)\tilde{n}(N-N^*)\tilde{n}(N^*)dN^*-\overline{\rho}\int_0^{\infty}\beta(N,N^*)\tilde{n}(N)\tilde{n}(N^*)dN^*$$
$$+\frac{\partial}{\partial N}\left[\overline{\rho}\dot{N}(N)\tilde{n}(N)\right]$$

The left-hand side of the PBE contains all the terms related to accumulation and transport of soot particles in the physical space, whereas the terms on the right-hand side represent, respectively, nucleation (or inception) of soot particles, rate of birth and death of new particles due to aggregation, and continuous rate of change of the number of primary particles per aggregate due to surface growth and oxidation (Zucca *et al.*, 2006).

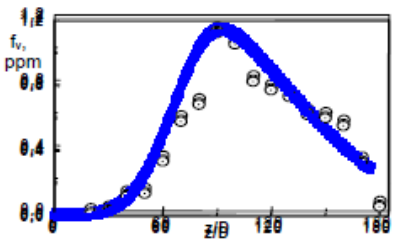


*Figure 1. Soot volume fraction at the flame axis: comparison between experimental data (points) and model prediction (line)*

The physical system investigated is a sooting turbulent non-premixed flame burning ethylene in atmospheric-pressure air (Hu *et al.*, 2003) and an example of the comparison between experimental data and model predictions along the flame axis is reported in Fig. 1

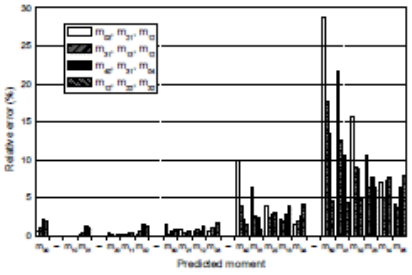


*Figure2: Relative errors for DQMOM (in comparison with Monte Carlo simulations) with N=2 on the predictions of some integer mixed moments with different choices for the sixth moment for a particulate system undergoing particle aggregation and sintering.*

In Fig. 2 the comparison for a bi-variate case of DQMOM predictions and Monte Carlo simulations is reported. In conclusion, our results show that DQMOM is a stable and accurate method for describing the evolution of a population of particles undergoing surface growth and oxidation, aggregation, and sintering and presents the great advantage of being computationally affordable and therefore can be easily implemented in CFD codes.

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