Multivariate Modeling of Soot Particles with the Hybrid Method of Moments

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A major challenge in soot modeling is the compatibility of an accurate physio-chemical description and computational efficiency. A promising approach to handle this trade-off are multivariate moment methods, which are based on moments of the soot Number Density Function (NDF). In this work, the Hybrid Method of Moments (HMOM) developed by Mueller *et al* (2009) is considered. HMOM is an easy to implement and computationally inexpensive, robust moment method that accounts for the experimentally observed bimodality of the soot NDF. It combines the Direct Quadrature Method of Moments (DQMOM) and the Method of Moments with Interpolative Closure (MOMIC). In the original bivariate model of Mueller *et al* (2009), soot particles are characterized in terms of two parameters, their volume (V) and their surface area (S). This model is referred to as VS-model. It is now demonstrated that HMOM can be extended to an arbitrary number of parameters.

Exemplarily, the generalization of HMOM is applied to a complex trivariate model (Blanquart and Pitsch, 2009b). The third independent parameter in this model is the number of active sites on the surface of the particles (H) which allows for characterization of their surface reactivity. With the VSH-model, the chemical processes of surface growth and oxidation can be described using not only the surface area, but also the number of active sites available for a reaction. The physical of processes nucleation, condensation, and coagulation can also influence the surface reactivity of the soot particles, and their formulation is therefore different from VS-HMOM. Originally, the VSH-model was integrated in DQMOM. While DQMOM is numerically less robust than HMOM, it is less restrictive for expressions that are allowed to occur in the moment source terms. These restrictions for HMOM require modifications in the formulation of the source terms, which are discussed in detail. An important example is the coagulation source term. In the original model, it is assumed that the surface reactivity $\chi = H/S$ is not changed due to coagulation, that is, a new particle of type $i+j$ formed by the collision of two particles i and j can be described by

$$\chi_{i+j} = \frac{H_{i+j}}{S_{i+j}} = \frac{H_i + H_j}{S_i + S_j}.$$

If this ratio is inserted in the coagulation source term, the resulting expression cannot be expanded into a finite sum of moments which is required for HMOM. Therefore, the description has to be modified. It is shown that the original trivariate model can be expressed in a way applicable in HMOM without abandoning the original chemical and physical ideas.

The multivariate HMOM is validated with an ethylene premixed flat flame at atmospheric pressure and a fuel-air-equivalence ratio of $\phi = 2.64$. This flame has been investigated experimentally by Xu *et al* (1997). As in MOMIC, HMOM allows different orders for the interpolative part of the closure approach. The new VSH-HMOM model is considered with a first order (P1) and a second order (P2) approach. The original VSH-model is integrated within Monte Carlo (MC) simulations. As shown on the left side in Fig. 1, all statistical frameworks allow an accurate prediction of the soot volume fraction.

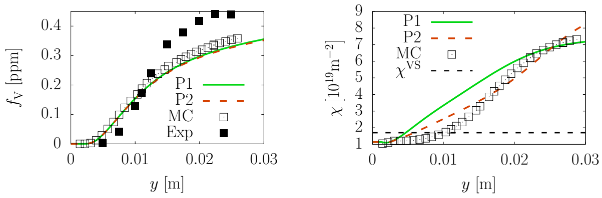

Figure 1. Predicted soot volume fraction (left) and surface reactivity (right). Experimental measurement by Xu *et al* (1997).

The MC simulations are also used as a reference to assess the accuracy of HMOM for the multivariate case and the impact of the required modifications for the source terms. A comparison of the surface reactivity is shown on the right side of Fig. 1. The surface reactivity can be important to capture temperature effects on the soot formation as shown by Blanquart and Pitsch (2009a). While the VS-model assumes a constant surface reactivity of $\chi^{\mathrm{VS}} = 1.7\times10^{19}\mathrm{m}^{-2}$, both the original and the new VSH-model predict an increase. The required modifications that allow HMOM as a numerically more robust framework do not introduce significant changes in the prediction of this quantity.

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