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Calculation of the size distribution function of soot particles in turbulent diffusion flames

Dirk Grosschmidt, Peter Habisreuther, Henning Bockhorn [*]

Engler Bunte Institut, Bereich Verbrennungstechnik, Universität Karlsruhe, Kaiserstrasse 12, 76128 Karlsruhe, Germany

Abstract

The advantages of a combined model approach were exploited to compute piloted natural gas/air turbulent jet diffusion flames with the intention towards a quantitative description of the soot properties (soot volume fraction) as well as the evolution of the size distribution of the soot particles across the flame. The interaction of turbulence and chemistry was described by a probability density approach in combination with the laminar flamelet formulation. Gas-phase chemistry was accounted for by the detailed mechanism of Appel, Bockhorn and Frenklach, which includes the formation of aromatic species up to pyrene. The formation and oxidation of the particulate phase was described by soot particle size population balance equations, which were solved using a modified version of the stochastic particle algorithm developed by Kraft and co-workers. The influence of turbulent fluctuations on particle inception, coagulation and surface reactions is discussed. The predictions of the particulate phase were assessed quantitatively by comparison with measurements of total soot particle concentrations of turbulent diffusion jet flames, which were investigated by Bartenbach et al. The evolution of the size distribution of the primary particles across the turbulent jet flame was visualized. After the region, where particle inception plays the dominating role, shape and extension of the size distribution is governed mainly by coagulation processes until the oxidation reactions are of increasing importance, leading to the consumption and depletion of particles, which significantly alters the distribution.
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1. Introduction

The quantitative description of soot in turbulent flames using numerical simulation is a valuable evaluation tool with potential in a wide range of technical applications (e.g. boilers, burners and combustors). In combination with CFD different approaches were followed to incorporate

soot formation into the prediction. These are either based on empirical correlations for the soot volume fraction f_v in combination with flamelet [1] and pdf methods [2], respectively, or on transport equations for f_v [3], where the source terms are calculated using the method of moments with interpolative closure [4]. The knowledge of integral properties such as soot volume fraction or total number density allow the comparison with measurements. With the development of techniques, that give access to the size distribution function by experiments [5], the demands towards the model efforts are rising. The knowledge of the

[*] Corresponding author. Fax: +49 721 608 7770.
E-mail address: henning.bockhorn@vbt.uni-karlsruhe.de (H. Bockhorn).

local particle size distribution allows conclusions regarding the morphology and the aggregation behaviour of the soot particles. This is a novelty in the context of soot predictions in turbulent diffusion flames. Up to now this information was available only for laminar configurations [6,7].

This paper is organized as follows: first the gas-phase model is described, then the averaged population balance equations and its unclosed expressions are discussed. After that results of turbulent jet flame calculations are shown and compared to measurements.

1.1. Flow field and gas-phase chemistry model

To calculate the averaged properties of the flow field a commercial 3D CFD solver was used in combination with a standard two equation turbulence model and a gradient diffusion formulation. The interaction of turbulence and chemistry was accounted for by solving an equation for the characteristic one-point, one-time Eulerian mass-weighted probability density function of the scalars, which describe the thermodynamical state of the flow. This evolution equation was solved using a Lagrangian particle approach, where the particles evolve by the diffusion process described in [8], page 187. The molecular mixing term was closed by the parametrized scalar profile (PSP) model, which was proposed by Meyer and Jenny [9], successfully validated against DNS data [9] and applied in simulations of the Delft flame [10] as a standard test case of a non-premixed flame. With its straightforward implementation and effectiveness with respect to computational time, the PSP model was adopted and evaluated for the present model application. Since the model has not been used in such an application yet, the model constants shall be given here. They are set as follows: $C_\kappa = C_\tau = 1$, $C_{\tau,\kappa} = 2$. Chemistry was described by the stretched laminar flamelet model [11,12] as it provides a way of including detailed chemistry to calculations of turbulent non-premixed flames. A drawback of the model is the assumption of a steady state within the structure of the laminar flamelet and the scalar dissipation rate, which is specified by the local state of the turbulent flow. Suggestions were made to overcome this matter and improve the model by accounting for transient effects [13,14]. However within this work the standard stretched laminar flamelet approach was used in order to reduce the complexity of the modeling effort at this point. Therefore, the thermodynamical state of the system is determined by the mixture fraction variable ξ and the scalar dissipation rate χ. ξ is defined as the sum of the element mass fractions of carbon and hydrogen, normalized with the conditions for pure fuel. The conserved scalar variable takes up the values 1—for pure fuel and 0—for pure air. The scalar dissipation rate χ is defined with the molecular diffusivity Γ as

$$\chi = 2\Gamma\left(\left(\frac{\partial\xi}{\partial x_1}\right)^2 + \left(\frac{\partial\xi}{\partial x_2}\right)^2 + \left(\frac{\partial\xi}{\partial x_3}\right)^2\right) \quad (1)$$

A thorough outline of the laminar flamelet model and the derivation of the governing equations is given, e.g. in [12]. For the turbulent flame calculations in this work flamelet libraries were generated based on the chemical mechanism presented by Appel et al. As it was outlined above, it includes well validated aromatic and soot precursor chemistry. Since χ varies through the flame, it is common to choose the value at the stoichiometric mixture fraction to characterize a laminar flamelet. Since the considered case is a turbulent jet flame, statistical independence of mixture fraction and scalar dissipation rate is assumed with the result, that the joint pdf is constructed by the product of the marginal pdfs [14]

$$\tilde{f}_{\xi\chi}(\hat{\xi},\hat{\chi};x_i) = \tilde{f}_\xi(\hat{\xi};x_i) \cdot \tilde{f}_\chi(\hat{\chi};x_i) \quad (2)$$

As proposed by various authors the scalar dissipation pdf is assumed to have the shape of a log-normal distribution, e.g. [14,15] with the parameters $\mu(x_i)$ and variance σ^2. The mean parameter $\mu(x_i)$ is related to mean quantities by $\mu(x_i) = \ln(\langle\chi(x_i)\rangle) - \frac{\sigma^2}{2}$, the variance σ^2 is assumed to be a constant ($\sigma^2 = 2.0$) in first approximation [15]. The mean of scalar dissipation rate is computed as a function of local mean quantities, i.e. the mixture fraction variance $\langle\xi''^2\rangle$ and the local turbulence frequency $\langle\omega\rangle$, which in turn is related to the turbulent kinetic energy $\langle k\rangle$ and the dissipation rate $\langle\varepsilon\rangle$ by $\langle\omega\rangle = \frac{\langle\varepsilon\rangle}{\langle k\rangle}$ and $\langle\chi\rangle = C_\chi\langle\omega\rangle\langle\xi''^2\rangle$, where C_χ is a model constant with the value of 2. The mixture fraction variance $\langle\xi''^2\rangle$ is retrieved from the local Lagrangian stochastic particle system, which represents the pdf of mixture fraction at point x_i, by computing the second central moment. Mean field estimates of dependent variables, e.g. species concentrations were technically computed by averaging over the pdfs of ξ and χ, see Eq. (3). This was achieved in mixture fraction space as the transported pdf variable by ensemble averaging over H intervals with the frequency h_n within the interval n. In χ-space a Romberg method was used to integrate the log-normal distribution

$$\langle\phi(x_i)\rangle = \int_0^1\int_0^\infty \phi(\xi,\chi;x_i)f(\chi)f(\xi)\,\mathrm{d}\chi\,\mathrm{d}\xi$$
$$\approx \frac{1}{H}\sum_{n=1}^{H'}h_n\cdot\int_0^\infty\phi(\xi_n,\chi;x_i)f(\chi)\,\mathrm{d}\chi \quad (3)$$

1.2. Model of the particulate phase

In this work the soot model developed by Frenklach and co-workers [16,17] is adopted. The model consists of a gas phase mechanism, which describes the oxidation reactions of the fuel