

# Aspects of Modeling Soot Formation in Turbulent Diffusion Flames

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## Introduction

The formation of soot in turbulent diffusion flames is a problem in combustion that is still not understood. In the past there have been two approaches to model this process using the laminar flamelet concept. The first approach was based on a flamelet library concept [1,2]. In this approach a flamelet library for the source terms of soot formation was generated. A transport equation for the soot volume fraction, that used the source terms from the library, was included in the CFD calculation. The second approach was based on instationary flamelet calculations, that were either done in interaction with the CFD calculation, or have been done in a post-process [3,4,5,6].

The flamelet library based method, has the advantage of very low computational cost when coupled with a computational fluid dynamics code as the method requires only the transport of two additional scalars, the mixture fraction and the mixture fraction variance. The interactive flamelet method has the advantage of not only including transient effects occurring in the soot formation processes, but also in the combustion process itself. Transient effects in the profiles of important intermediate species, such as radicals and soot precursors, may have a significant impact on the source terms of particle inception, surface growth or oxidation. Therefore in this work, the representative interactive flamelet approach is chosen in order to provide a reference case for further validation of the flamelet library based soot model.

## The Experimental Test Flame

As in [2] we use the experiments by Young et al. [7] on a rim-stabilized ethylene turbulent jet diffusion flame. Ethylene is injected through a pipe with a diameter of 3.1 mm at a speed of 24.5 m/s into stagnant air at room temperature and atmospheric pressure. The soot volume fraction was measured by laser absorption along with mixture fraction by microprobe sampling, and temperature by fine wire thermocouples.

## The Detailed Kinetic Soot Model

The detailed kinetic soot model follows the approach by Mauss [8]. During the oxidation of the hydrocarbon fuel, aromatic species are formed in the gas phase of the flame and grow to poly-aromatic structures. Species with more than four rings can combine and incept soot particles [9]. They can further condense on the soot particle surface and contribute to the surface growth process. Soot particles collide and, depending on their size and the surrounding environment, combine to larger spherical particles or to agglomerates [10]. All these processes can be calculated from the Smoluchowski equation. In addition heterogeneous surface growth and oxidation reactions are taken into account. The surface growth is modeled by the simple hydrogen abstraction carbon addition mechanism (HACA) [11]. Oxidation occurs via reactions of OH and O<sub>2</sub> on the soot particle surface. Further details of the soot model can be found in [8,12]. In addition to the model in [8], the agglomeration model by Frenklach et al. [13] was added. For the reference calculation the fractal dimension

of the particles was kept constant  $D_f = 1.8$ . The chemical mechanism for the gas phase and for the heterogeneous surface reactions was also taken from [8]. The rate coefficients were however slightly changed, with the major difference being the reduction of the reaction rate coefficients for the oxidation reactions. The oxidation reactions are more sensitive in diffusion flames, which are under consideration here, than in premixed flames that were under consideration in [8].

### **Instationary Flamelet Modeling**

Soot formation in turbulent diffusion flames was recently investigated by Pitsch et al. [14]. In this publication it was concluded that, it is necessary to include preferential diffusion effects for soot particles, to be able to predict the measured profiles for the soot volume fraction in a turbulent ethylene-air jet diffusion flame. We found, however, that the predicted profile for the soot volume fraction is very sensitive on a number of parameters that were not investigated in the previous study [14]. In this contribution we investigate parameters other than preferential diffusion and use the unity Lewis number simplification.

The parameters we investigate are the choice of the dependence of the scalar dissipation rate on the mixture fraction, and the influence of agglomeration processes. To describe the dependence of scalar dissipation on mixture fraction ( $Z$ ) we use an inverse complementary error function defined between  $Z=0$  and  $Z=Z_{\max}$ , where  $Z_{\max}$  is chosen to be the mean of the mixture fraction on the centerline of the turbulent diffusion flame. The scalar dissipation rate is calculated from the conditional mean scalar dissipation rate at the position of maximum scalar dissipation in  $Z$ , allowing calculating the instationary flamelet at heights, where the maximum mixture fraction is less than the stoichiometric mixture fraction. The conditional mean scalar dissipation rate is calculated as suggested in [3].

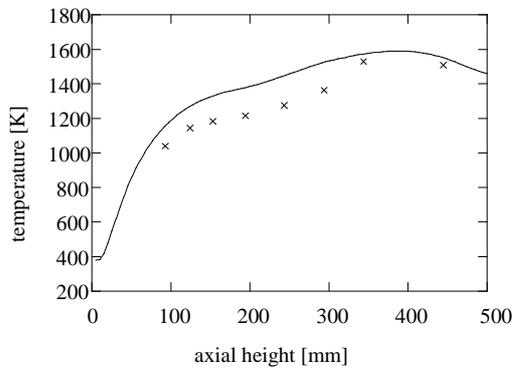
To investigate the effect of agglomeration we use the agglomeration model from Ref. [13].

### **Results and Conclusion**

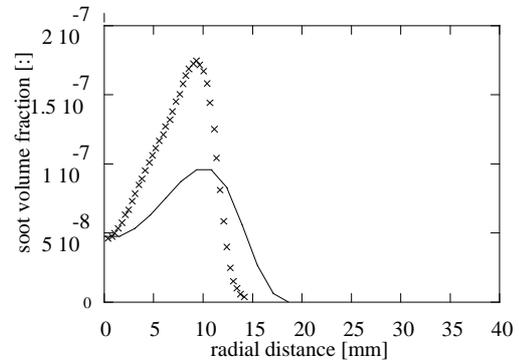
The calculated axial temperature profile at the centerline is shown in **Figure 1**. It can be seen that the calculated temperature in the core of the flame is up to 200 K higher than found in the experiment. The mixture fraction becomes stoichiometric at a height of 350 mm. From this height the calculated temperature profile is in agreement with the experiments. The same can be concluded for the comparison between numerical calculation and the experiment of the radial temperature profile shown in **Figure 2**. At a height of 160 mm is the predicted temperature in the core of the flame about 200 K higher than the experimental. Calculation and prediction agree for stoichiometric and fuel lean conditions. The results calculated from instationary flamelets are consistent with the results in [2], where a flamelet library was used. It is worthwhile to mention that temperature measurements with thermocouples in the core of a sooting turbulent diffusion flame are difficult to perform. The numerically calculated profiles for the soot volume fraction are compared with the experimental data in **Figure 3- Figure 6**. The shape and the height of the predicted profiles in **Figure 3** agree well with the experimental data. The maximum in the predicted soot volume fraction is lower than in the experimental data. This is most probably caused by an inaccuracy in the predicted mixture fraction field. The mixing occurs in the simulation faster than in the experiment. This can also be seen in **Figure 5** and **Figure 6**. It appears that the shape of the predicted and experimental profiles agree well. However, the numerical profiles are narrower.

Other than in [14], a good agreement between calculation and experiment could be found, without assuming preferential diffusion of soot. We found that there is a permanent loss of

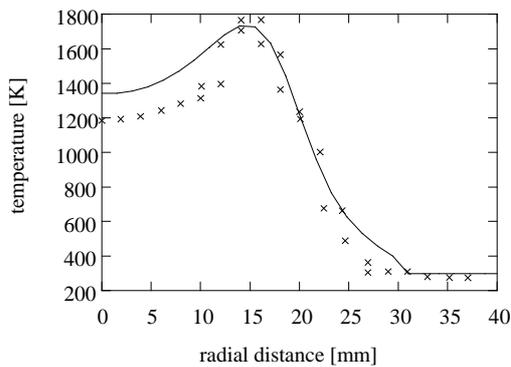
soot in the instationary flamelet model, if the decrease of the maximum mixture fraction, needed in the formulation of the scalar dissipation rate is not taken into account. The inclusion of the maximum mixture fraction  $Z_{\max}$  causes that the scalar dissipation rate becomes zero at  $Z=Z_{\max}$ , causing that the diffusive terms in the flamelet equations become zero for  $Z=Z_{\max}$ .



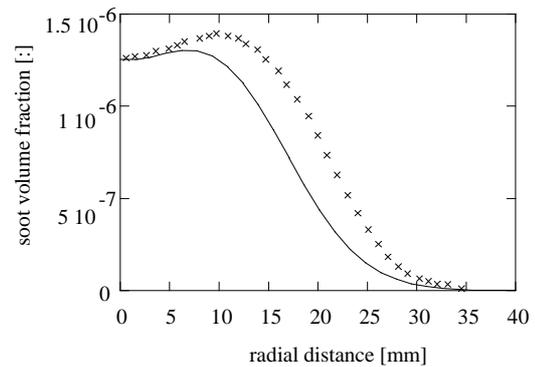
**Figure 1.** The axial temperature profile.



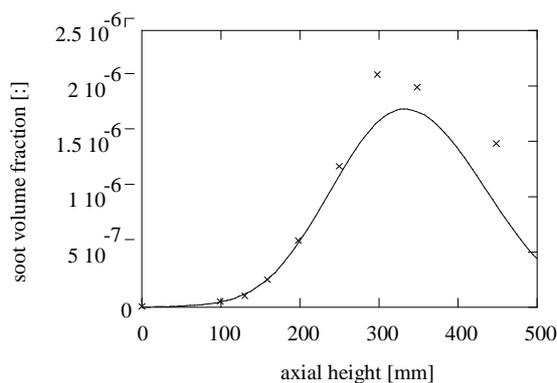
**Figure 4.** The radial soot volume fraction at a height of 100 mm.



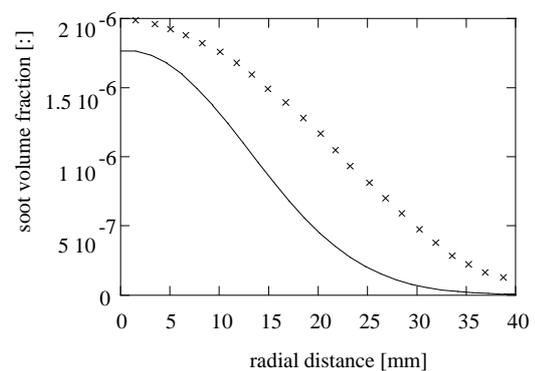
**Figure 2.** The radial temperature profile at a height of 160 mm.



**Figure 5.** The radial soot volume fraction profile at a height of 250 mm.



**Figure 3.** The axial soot volume fraction profile.



**Figure 6.** The radial soot volume fraction profile at a height of 350 mm

## References

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