Pollution Formation in Turbulent Non-Premixed Combustion Using Different Flamelet Models

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It is of engineering interest to find simple but valid models capable to describe the formation and oxidation of soot in turbulent jet diffusion flames. As shown before, such a model can be obtained in the framework of the laminar flamelet library concept [1], [2]. A detailed chemical soot model is applied to calculate the libraries containing the rates of soot particle inception, soot volume dependent surface growth and oxidation as well as species and temperature fields. A transport equation for soot is solved in the CFD-code that uses the sources tabulated in the library. Flame radiation can be taken into account if an additional parameter is introduced, describing how long time the radiation acted on the flamelet [3].

Various formulations of the laminar flamelet model are given in literature. In previous work the effects of differential diffusion and variation of scalar dissipation rate on the flame structure has been investigated [4]. In this work we study how a change in the modelling of species diffusion influences the calculated appearance of soot in a turbulent non-premixed ethylene-air flame. The source terms of soot are computed and tabulated for three different flamelet models. They are defined using various modifications of the species diffusion term and the term containing the specific heat in the formulation. The libraries are used to calculate a turbulent jet diffusion flame and the results are compared with each other and corresponding experiments [5].

The formation of soot is a slow chemical and physical process and equilibrium conditions can not be reached in flame configurations with time- and length-scales relevant for engineering applications. The assumption of a quasi-steady burning state, which the flamelet library concept is based on [6], is therefore not valid for soot. Instead, the unsteady transition of the flamelet must be calculated in interaction with the CFD-calculation [7]. The computational effort of this method is high. Our concept to calculate the formation of soot in interaction with a CFD-code, taking source terms of soot from laminar flamelet calculations, is an efficient approximation of the transient process of soot formation. Another transient process, the heat loss of the flame due to radiation, is modeled as explained in ref[8]. The efficiency of the concept could be further increased by approximating the library with non-linear curve fits. The influence of preferential diffusion on inception, growth and oxidation of soot is investigated in this abstract. We therefore introduce three different models:

•**Model 1:** We assume that the Lewis numbers of the species are constant. They are considered to be unity for all species except for H and H_2. This could model the appearance of preferential diffusion in a thin layer around the stoichiometric mixture fraction.

•**Model 2:** Here we apply unity Lewis numbers for all species. The assumption implies that the main mixing process is turbulent and that the turbulent Lewis numbers are equal to one.

•**Model 3:** A complex diffusion model is applied for all species. Preferential diffusion is taken into account.

Figure 1 shows the rates of soot particle inception a), soot surface growth b) and soot oxidation c) as functions of the mixture fraction for a scalar dissipation rate at stoichiometric mixture $\chi_{st} = 0.01\ [1/s]$ for the three models. This low scalar dissipation rate has been chosen since it is relevant in most part of the flame (ref[8]).The soot flamelet libraries are calculated for all models. This is done by computing laminar counterflow diffusion flames in a Moore-Steward transformed coordinate system. A mixture fraction transport equation is calculated together with the other transport equations. The stoichiometric mixture fraction has been chosen to be the mixture fraction at maximum temperature. The soot model applied has been taken from ref. [8] without any changes. The source terms are read by the CFD-code simulating the turbulent diffusion flame. We employ experimental data from the literature for validation. Young et al. [5] carried out the experiments on a rim-stabilized ethylene turbulent jet diffusion flame. The comparison of the calculated mixture fraction and temperature is shown in Figure 2.

Results are shown for the calculation applying the library of Model 2. The agreement with experiments and calculation in the axial and the radial profile are good. It can be seen from figure 3 that the calculations with unity Lewis number (Model 2) and with the complex diffusion model (Model 3) results in much to low soot volume fraction. The calculation with Model 1 including H and H_2 gives soot volume fractions near to the experimental data. However the calculated axial profile is shifted 50 mm down stream compared to the experiments. We find that Model 1 gives the best agreement with the experiment. The soot oxidation occurs too late in all models, but Model 1 reaches a maximum mean value, which is very close to the values found in experiments.

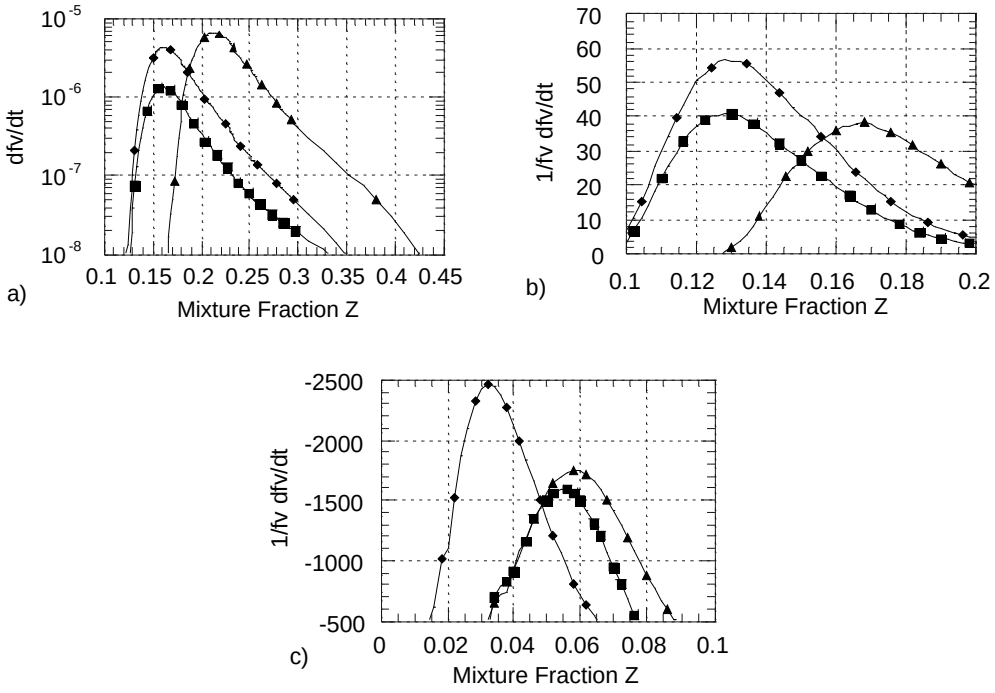

Figure 1: Rates of soot formation a) particle inception, b) surface growth and c) oxidation in dependence on the mixture fraction Z with χ_{st} =0.01 $[1/s]$. Compared are Model 1♦, Model 2 ■ and Model 3▲.

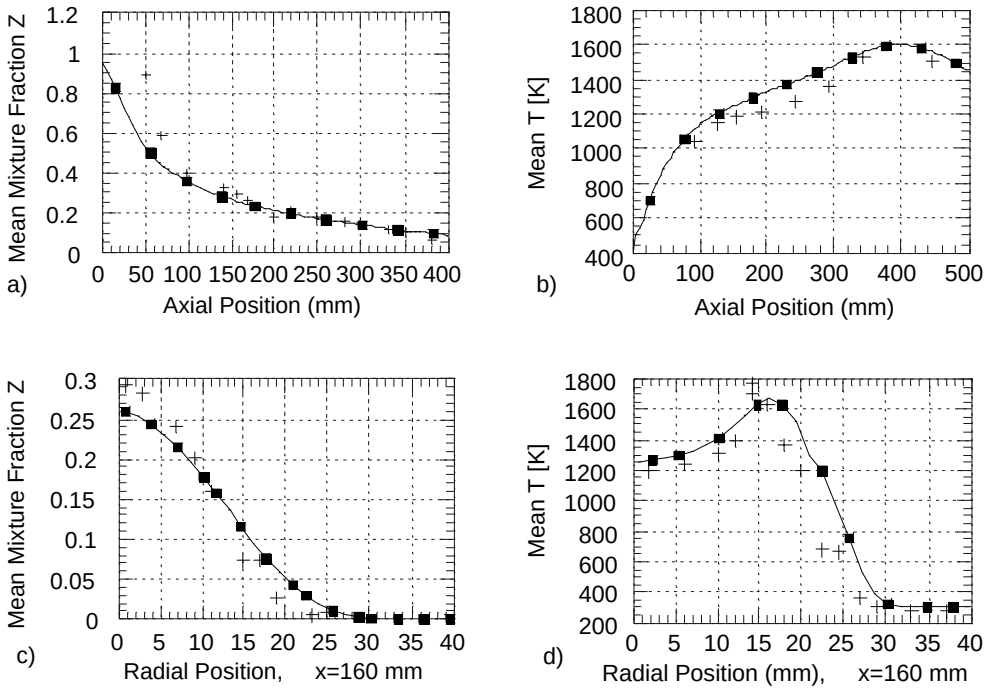

Figure 2: Mixture fraction and temperature as a function of axial [a), b)] and radial [c), d)] position. Comparison of Model 2■ and experimental data +. Figure a) shows a shift in mixture fraction of 50 mm of experimental data and computation close to the outlet on axis.

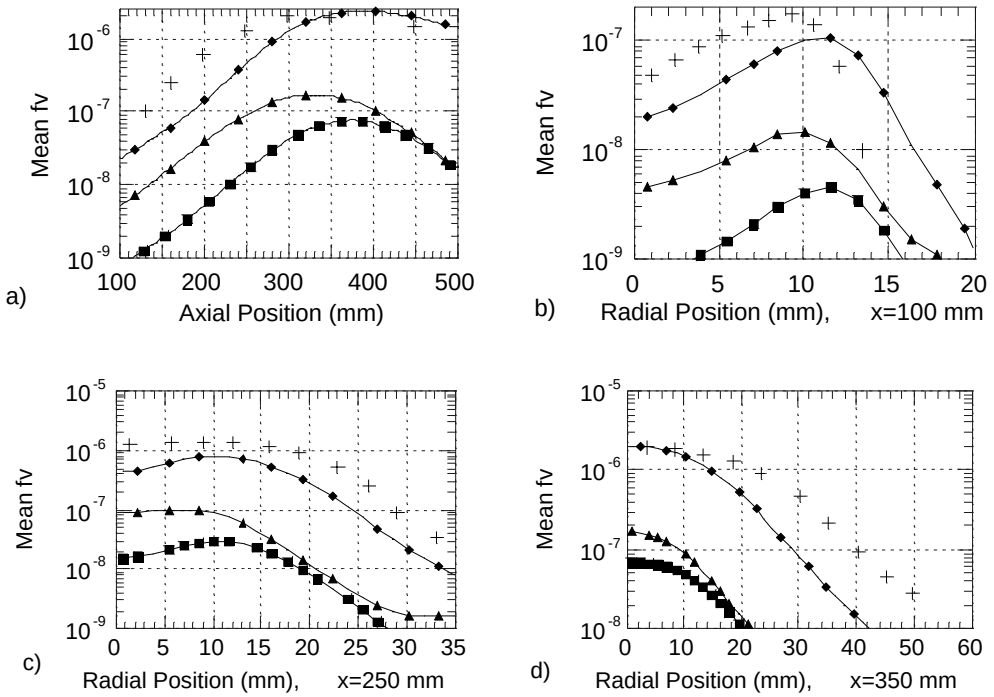

Figure 3: Soot volume fraction as a function of axial position a), radial position at a distance of 100 mm b) 250 mm c) and 350 mm over the burner. A comparison of experiments +, Model 1 ♦, Model 2 ■ and Model 3▲.

Acknowledgment

This work has been partially supported by the Swedish Center of Strategic Research in Combustion Science and Technology CeCoST.

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