

Predicting and measuring soot formation and particle size distributions in a laminar diffusion flame

C.E. Garcia-Gonzalez¹, F. Sewerin¹, A. Liu¹, S. Rigopoulos¹, B.A.O. Williams^{1,2,*}

¹ Department of Mechanical Engineering, Imperial College London

² Department of Engineering Science, University of Oxford

Abstract

We present the results from a joint experimental and modelling investigation of a laminar diffusion flame on a Santoro burner. The experimental techniques include laser diagnostic measurements and extractive thermophoretic sampling. In order to predict the spatial evolution of the primary soot particle size distribution throughout the flame, we employ a detailed population balance model. From the model predictions, “modelled” laser diagnostic signals are obtained which we directly compare with the experimental laser diagnostic images. This allows us to assess the validity of the model with reduced uncertainty by reducing the set of assumptions commonly made when recovering physical magnitudes from experimental signals.

Introduction

Soot is both an undesired product of hydrocarbon combustion and an air pollutant which causes adverse health effects. For this reason, the soot formation process has been the focus of continuous research since the 1960s [1, 2], with the double purpose of reducing emissions and understanding why these nanoparticles form. The difficulty in understanding and modelling soot formation can be related to the interaction of four main processes: chemical kinetics, controlling the reaction rates and the production of precursor species; particle inception, defining how protoparticles nucleate from a fluid; particle growth, including surface growth and coalescence; and a post-growth stage involving agglomeration and particle size reduction by oxidation. In order to investigate these processes, analyses are frequently carried out on laminar diffusion flames since they provide geometrically simple, accessible and reproducible model systems. Examples for such model systems are the flames originally investigated by Santoro et al. [3, 4]. Although several mechanisms of soot formation have been proposed [5–7], models still tend to underpredict both the soot volume fraction and the mean particle size on the centreline of laminar diffusion flames [8].

Specific Objectives

The scientific contribution of our work is threefold: First, we present OH-LIF and soot-ELS measurements characterizing a laminar diffusion flame on the Santoro burner and analyze TEM images of thermophoretically sampled soot particles regarding the distribution of primary soot particle sizes. Second, we apply a recently developed explicit adaptive grid discretization scheme in order to solve a population balance model that was previously developed within our research group for predicting the evolution of the soot particle size distribution in the investigated flame. Finally, based on the modelled

gas phase composition and particle size distributions we deduce predictions of the OH-LIF and ELS signals for comparison with the experimentally recorded signals.

Experimental Setup

A co-flow diffusion burner with an 11.1 mm ID nozzle raised 4 mm over a 101.6 mm diameter co-flow was used (Figure 1). A test case with an ethylene flow rate of 4.08 cm³/s and an air co-flow of 713 cm³/s was considered. During the measurements, the flame was shielded from ambient air currents by a chimney. Except for the slightly higher fuel flow rate, our flame configuration corresponds to ‘Experiment 1’ of Santoro et al. [3] and ‘Experiment 2’ of Santoro et al. [4]. In the investigation, two laser diagnostic techniques were employed: elastic light scattering (ELS) and laser-induced fluorescence (LIF), supplemented by thermophoretic sampling (TPS). Here, the ELS signal originates from two main contributions: molecular scattering and particle scattering. If the primary particle diameter is much smaller than the wavelength of the incident light, the ELS signal from the particles scales with the sixth power of the particle diameter such that, in comparison, the molecular contribution to the ELS signal becomes negligible.

A Q-switched frequency-doubled Nd:YAG laser was used in conjunction with sheet-forming optics to illuminate a 23 mm × 100 μm region across the burner centreline. The ELS signal was collected using a CCD camera with a 105 mm f/16 lens at 90° to the laser beam. The laser energy per-shot was attenuated to 0.5 mJ in order to avoid CCD saturation. Additional measurements were performed by vertical translation of the burner. Postprocessing included background subtraction, intensity correction and beam profile correction.

The Nd:YAG laser was also used to pump a frequency-doubled Rhodamine 6G dye laser tuned to 283.6 nm to excite the $Q_1(8)$ ($v = 1 \leftarrow 0$) transition in the $A^2\Sigma \leftarrow X^2\Pi$ electronic system of the OH radical. This transition has been chosen so that the LIF signal is only weakly sensitive to temperature. The fluores-

*Corresponding author: benjamin.williams@imperial.ac.uk
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cence signals from the ($\nu = 0 \leftarrow 0$) and ($\nu = 1 \leftarrow 1$) branches were collected with a gated intensifier and a CCD camera. Strong broadband fluorescence attributed to PAH species was detected in addition to fluorescence from the OH radical. The two fluorescence signals were separated by subtracting the signal detected when the laser is detuned from the OH spectral line from the signal recorded when the laser is tuned. Laser energy and sheet thickness were adjusted to ensure operation inside the linear LIF regime. Background subtraction, intensity correction and beam profile correction were subsequently performed, assuming the flame is optically thin and neglecting quenching effects.

Particle samples were obtained using a thermophoretic sampling device similar to that described by Dobbins and Megaridis [9]. Here, a double-action pneumatic cylinder introduces a 3 mm holey carbon TEM grid into the flame, retracting it after a pre-set residence time of 120 ms. The grid was held vertically during sampling in order to minimize disruption to the flow. Samples were analysed in a Jeol 2100+ transmission electron microscope (TEM) at an acceleration potential of 200 kV without additional preparation and images exported to *Image-J* for primary particle sizing.

Modelling approach

Following a common practice, we describe the reacting gas phase in terms of n reactive scalars $\mathbf{Y}(\mathbf{x}) = (Y_1(\mathbf{x}), \dots, Y_n(\mathbf{x}))$ representing the species mass fractions and the mixture enthalpy. Within the ambient flow, the reactive scalars evolve according to

$$\sum_{j=1}^3 \frac{\partial \rho u_j Y_i}{\partial x_j} = \sum_{j=1}^3 \frac{\partial}{\partial x_j} \left(D_i \frac{\partial Y_i}{\partial x_j} \right) + \dot{\omega}(\mathbf{Y}), \quad (1)$$

$i = 1, \dots, n$, where $\mathbf{u}(\mathbf{x})$ represents the ambient velocity field, $\rho(\mathbf{x})$ is the mixture density, $D_i(\mathbf{Y}(\mathbf{x}))$ denotes the diffusivity of scalar i into the mixture and $\dot{\omega}(\mathbf{Y}(\mathbf{x}))$ are the scalar production or destruction rates.

Eq. (1) is complemented by the continuity and momentum conservation equations for a Newtonian fluid. The equation of state and all constitutive relations describing the fluid are those associated with an ideal gas. Considering ethylene as fuel, we employ the comprehensive USC II reaction mechanism [10]. The reduction in mixture enthalpy as a result of radiation from gas phase H_2O , CO_2 , CH_4 and CO and from soot is computed based on the assumption of optical thinness of the flame [11]. In this regard, the Planck mean absorption coefficients are obtained in terms of temperature from approximating polynomials [12].

For the immersed soot particle phase, on the other hand, we adopt a continuum description based on the so-called population balance equation [13]. Physically, the latter represents a balance law governing the particle number density $N(l, \mathbf{x})$ which evolves both in physical

space ($\mathbf{x}$) and in particle size space (l).

$$\sum_{j=1}^3 \frac{\partial (u_j + v_j) N}{\partial x_j} + \frac{\partial G(l, \mathbf{Y}) N}{\partial l} = \dot{s}(l, N, \mathbf{Y}) \quad (2)$$

Here, $\mathbf{v}(\mathbf{x})$ represents the thermophoretic particle velocity [14, Eq. (39)₁] and $G(l, \mathbf{Y}(\mathbf{x}))$ denotes the particle growth/oxidation rate, while the source term $\dot{s}(l, N(l, \mathbf{x}), \mathbf{Y}(\mathbf{x}))$ indicates the soot nucleation rate. Our observations based on TEM imaging of thermophoretically sampled soot particles (see Figure 7 below) suggest that the primary soot particles can be approximated as spheres with diameter l . Although the TEM images further indicate that soot particles tend to assemble in the form of grape-like aggregates, we do not include any physical description of the aggregation process at present. Conceptually, this is tantamount to replacing an aggregate by a loose collection of its constituting primary particles. Since this simplification does not influence the flow or primary particle formation dynamics, we do not expect any negative impact on our predictions of primary particle size distributions due to the omission of aggregation. However, Ivezic and Menguc [15] argued that the contribution of an aggregate to the local ELS signal is comparable with the signal emitted by a single spherical particle whose radius coincides with the aggregate's radius of gyration. By consequence, our reduction of aggregates to disjointed primary particles is expected to entail an underprediction of the ELS signal.

The kinetic nucleation and growth rates in Eq. (2) are based on acetylene C_2H_2 and have previously been employed within our research group to predict soot formation in the Santoro flame series [16] as well as a turbulent methane-air diffusion flame [16, 17]. Following Liu et al. [18], the soot nucleation rate is given by

$$\dot{s}(\mathbf{Y}) = \frac{2N_A}{C_{\min}} [\text{C}_2\text{H}_2] k_1(T), \quad (3)$$

where angled brackets represent molar concentrations, N_A is Avogadro's number, $C_{\min} = 700$ denotes the number of carbon atoms in a soot nucleus and $k_1(T)$ is given by $k_1(T) = 1.7 \exp(-7548 \text{ K}/T) (s^{-1})$. The cumulative particle growth rate, can be computed from

$$G(l, \mathbf{Y}) = \frac{2}{\rho_s} (s_{\text{C}_2\text{H}_2}(\mathbf{Y}) - s_{\text{OH}}(\mathbf{Y}) - s_{\text{O}_2}(\mathbf{Y})), \quad (4)$$

where $\rho_s = 1900 \text{ kg/m}^3$ is the density of solid soot and the surface-specific growth and oxidation rates [18] are given by

$$s_{\text{C}_2\text{H}_2}(\mathbf{Y}) = 2p_{\text{C}_2\text{H}_2} k_2(T), \quad (5)$$

$$s_{\text{OH}}(\mathbf{Y}) = 167 \frac{p_{\text{OH}}}{\sqrt{T}}, \quad (6)$$

$$s_{\text{O}_2}(\mathbf{Y}) = 1200 p_{\text{O}_2} \left(\frac{K_A(T) \chi}{1 + K_z(T) p_{\text{O}_2}} + K_B(T) \chi' \right) \quad (7)$$

and

$$\chi = \left(1 + \frac{K_T(T)}{K_B(T) p_{\text{O}_2}} \right)^{-1}, \quad \chi' = 1 - \chi. \quad (8)$$

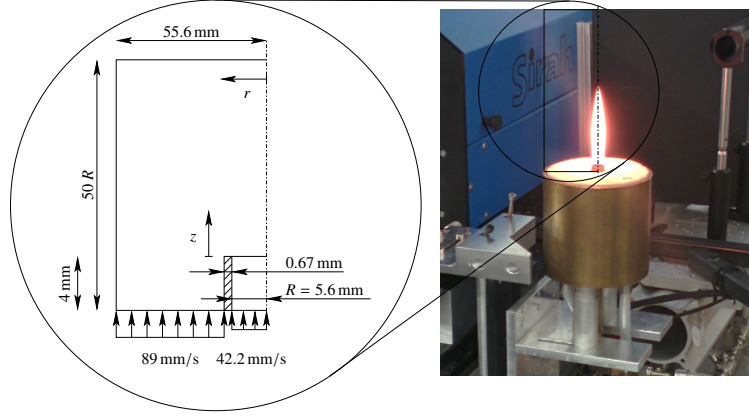


Figure 1: Photograph of the non-smoking flame investigated in this work (right) and schematic illustration of the computational domain (left).

In Eqs. (5) through (7) $p_{C_2H_2}$, p_{OH} and p_{O_2} denote partial pressures (in [atm]), $k_2(T)$ reads $k_2(T) = 470 \exp(-16004 \text{ K}/T)(s m^{-1})$ and $K_A(T)$, $K_z(T)$, $K_B(T)$ and $K_T(T)$ are specified by Nagle and Strickland-Constable [19, p. 162].

Mueller et al. [20] point out that incipient soot particles have a liquid-like consistency and may hence contribute to coalescent growth by merging with other incipient particles or by ‘splashing’ onto larger carbonized particles. For the purpose of the present work, this effect is neglected. According to Liu et al. [18], it is not the main contributor to the overall soot yield and may only be significant in the soot nucleation regions of a flame.

The inception and growth or destruction of soot particles is counterbalanced by source or sink terms in the scalar transport equations. These terms are based on the nucleation rate in Eq. (3) and the specific growth and oxidation rates in Eqs. (5) through (7) as well as the stoichiometry of the nucleation, growth and oxidation reactions. For more details we refer to Hall et al. [14].

The model equations presented above are reformulated in cylindrical coordinates and solved numerically on the domain depicted in Figure 1 using our in-house software LES-BOFFIN [21] adapted for laminar flows. The spatial grid in the r - z domain encompasses 100×200 finite volume cells. For the discretization of the PBE in l -space, $l \in [l_{\min} = 2.4 \text{ nm}, l_{\max} = 10 \mu\text{m}]$, we apply the explicit adaptive grid approach recently proposed by Sewerin and Rigopoulos [22] using 50 finite volume cells with a minimum node density of 4 nodes in $[l_{\min}, l_{\max}]$ and a maximum grid stretching of $r = 4$.

Results and Discussion

In this section, we present comparisons of the numerical solution of our model with experimental measurements both reported by Santoro et al. [3, 4] and laser diagnostic measurements obtained by us within the scope of this work. Here, we include a comparison with the existing experimental data (albeit obtained for a flame with a slightly smaller volumetric fuel flow rate) in order to indicate the similarity of our predicted

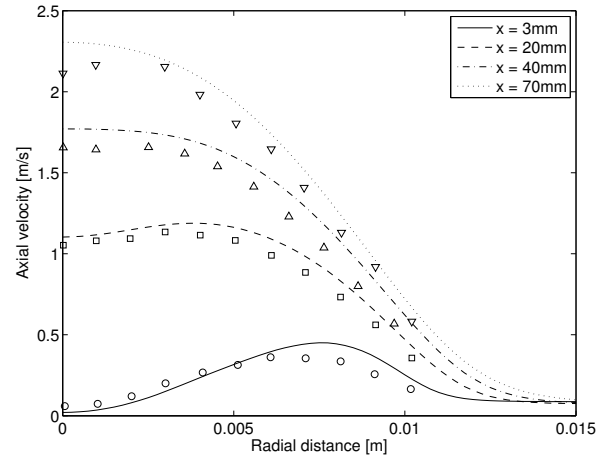


Figure 2: Comparing model predictions of the radial profiles of axial velocity (lines) with measurements of Santoro et al. [4] (symbols).

velocity and temperature fields with those of the non-smoking flame originally investigated by Santoro et al. [3, 4]. This may be viewed as a ‘calibration’ of our investigated flame against its blueprint counterpart.

Figures 2 and 3 depict comparisons of radial profiles of axial velocity and temperature, respectively, with the measured data of Santoro et al. [4] at several axial measurement stations. The velocity profiles are slightly overpredicted and, similarly, the predicted temperature profiles seem to be attained slightly upstream in the flame sketched by the temperature measurements. This reflects the slightly increased volumetric fuel flow rate in our configuration and indicates that, by consequence, the predicted flame seems longer than the measured. (Observe, for instance, the final temperature profile.)

Referring again to the measurements of Santoro et al. [3, 4], profiles of the radially integrated soot volume fraction are compared in Figure 4. These profiles characterize the overall soot yield in the flow direction and allow for the distinction of regions in which soot nucleation and growth or oxidation are dominating. Although the predicted and measured profiles slightly dif-

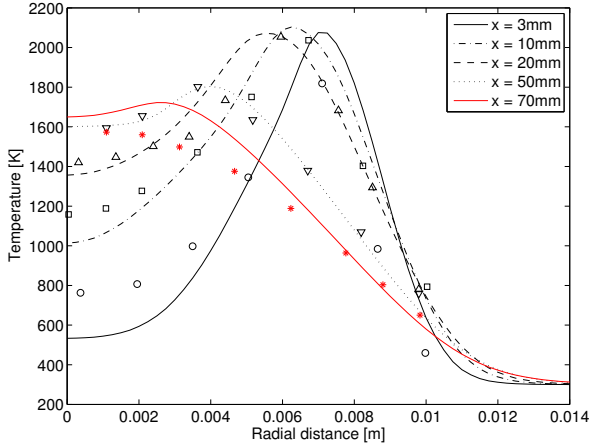


Figure 3: Comparing model predictions of the radial temperature profiles (lines) with measurements of Santoro et al. [4] (symbols).

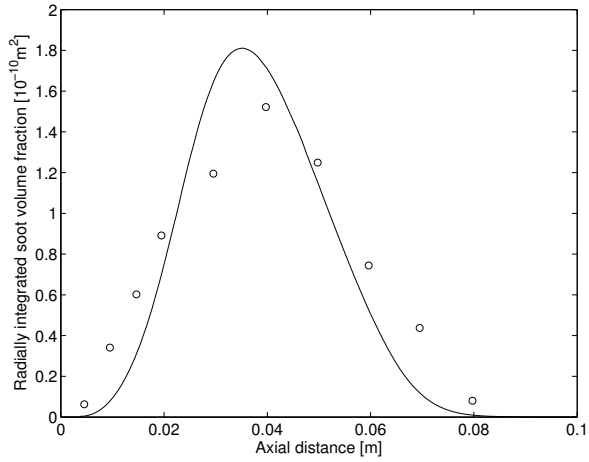


Figure 4: Comparing model predictions of the integrated soot volume fraction along the centreline (solid line) with measurements of Santoro et al. [3] (symbols).

fer in shape near the nozzle exit plane and close to the flame tip, the amount of soot formed and oxidized is well predicted. The maximum soot yield is slightly overpredicted and, although soot formation by volume is slightly delayed in the near field, soot oxidation sets in slightly too rapidly further downstream. We believe that these discrepancies are, at least in part, related to the observation that most of the soot particles are predicted to be formed in the wings of the flame, while the centreline soot is underpredicted by over an order of magnitude (see Figure 5 below). In turn, we suspect this to be caused by the acetylene-based soot kinetics.

Figure 5 depicts contour plots of the normalized OH-LIF and ELS signals both recorded experimentally and predicted by our model. Assuming the flame is optically thin and neglecting quenching, the OH-LIF signal is proportional to the molar OH concentration [23],

$$\text{OH-LIF} \propto [\text{OH}], \quad (9)$$

while the light scattered elastically by soot is related to the square of particle volume, modelled as the sixth mo-

ment of the primary particle size distribution [24],

$$\text{ELS} \sim M_6(\mathbf{x}) = \int_{l_{\min}}^{l_{\max}} l^6 N(l, \mathbf{x}) dl. \quad (10)$$

In Figure 5, the individual frames obtained from the laser diagnostic measurements do not stitch perfectly to provide coherent and smooth contour plots. This may be due to the sensitivity of the flame to ambient air currents entering through the chimney's windows or the slightly different flame topology on different days or times on a day. At least in part, we believe this to be related to the humidity in the laboratory air which could not be controlled during the experiments and, potentially, due to varying ambient laboratory temperatures. Qualitatively, the predicted and measured reaction zones indicated by the OH concentration correspond well, although the predicted flame appears to be vertically longer than suggested by the OH-LIF measurements.

Despite the reasonable agreement between the predicted ELS signal distribution and the measured one, we wish to comment on two major differences. On the one hand, the width of the flame wings in which most of the soot (by volume) is concentrated is slightly overpredicted. On the other hand, the ELS measurements indicate a notable amount of soot on the centreline between the wings which is completely absent in the model prediction. In view of our reasoning above, both of these points may be related to a limitation of the acetylene-based soot kinetics. The second point may further be enhanced by our omission of an aggregation model.

For a quantitative comparison, we consider radial profiles of the predicted and experimentally recorded ELS signals at two axial measurement stations in Figure 6. At the first measurement station, the profiles correspond well in shape and magnitude, but appear radially shifted apart by approximately 1.5 mm. Here, the experimental measurements suggest that the flame wings are located further towards the centreline of the flame. A similar shift can be observed at the second measurement station downstream. Following previous observations, the measured ELS signal indicates scattered light stretching from the wing towards the centreline which is not reproduced by the predicted ELS profiles.

In order to assess the influence of the soot polydispersity on the predicted ELS signal, we also computed the ELS signal assuming a monodisperse particle population with the population size at each spatial location given by the mean particle diameter $l_{10}(\mathbf{x})$,

$$l_{10}(\mathbf{x}) = \frac{M_1(\mathbf{x})}{M_0(\mathbf{x})}. \quad (11)$$

In Eq. (11), $M_0(\mathbf{x})$ and $M_1(\mathbf{x})$ represent the zeroth and first moment of the particle size distribution, respectively. The corresponding radial profiles are shown as red lines in Figure 6 and almost perfectly overlap with the radial ELS profiles computed based on the complete soot size distribution at each spatial location. This

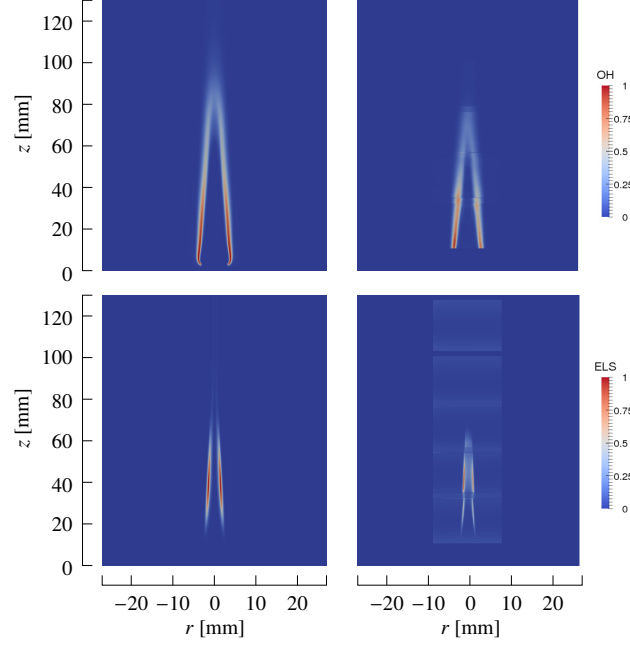


Figure 5: Comparing model predictions of the normalized OH LIF ($\sim [\text{kmol}/\text{m}^3]$) and ELS ($\sim [(\text{m}^3)^2/\text{m}^3]$) signals (left) with the experimental signals (right). The slight asymmetry of the measured contour plots is related to an attenuation of the laser beam which enters from the left hand side.

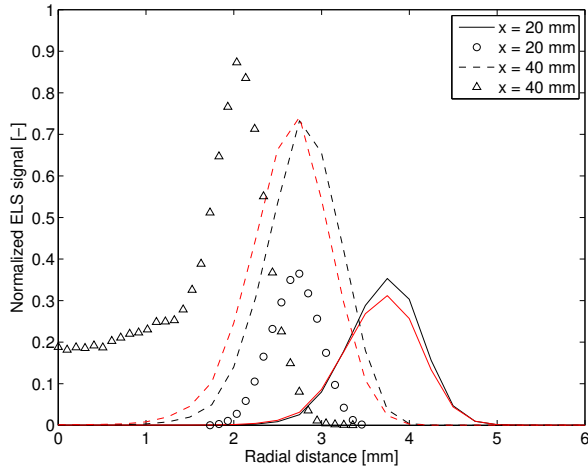


Figure 6: Comparing radial profiles of the computed ELS signal (black lines) with the experimentally recorded signal (symbols). Here, the red lines indicate the radial profiles obtained by assuming a locally monodisperse particle size distribution.

match also extends to other radial profiles and, with minor discrepancies, to the whole flow domain. We conclude that, at least in this flame, the polydispersity of the soot particulate phase does not influence the modelled ELS intensity and that for the purpose of obtaining a measure of particle size from experimentally recorded ELS images a monodisperse assumption is justified.

Figure 7 shows TEM images of soot particles which were thermophoretically sampled at different heights above the nozzle on the centreline. Our images suggest a change in morphology similar to Kholghy et al. [25]: Almost no particles are detected at 10 mm, while loose

liquid-like particles that are thought to be nano-organic carbon particles [26] appear at 20 mm. Further downstream, at 30 mm, most of the soot exists in the form of large aggregated solid particles. These particles significantly shrink in size due to oxidation as we move to 40 mm. Commensurate with the decay of the ELS signal, no particles are detected for heights above 50 mm.

Based on TEM images of thermophoretically sampled soot particles on the centreline, we also obtained estimates of the mean and standard deviation of primary soot particle diameters. Figure 8 depicts the change in mean particle diameter along the centreline of the flame. Here, quantitatively reasonable agreement is only attained between 40 mm and 60 mm above the nozzle exit plane. While the contour plots of the modelled soot nucleation and growth rates indicate that in this region soot formation has not ceased yet, our TEM images suggest that soot oxidation is dominant instead. The error bars in Figure 8, moreover, indicate the change in standard deviation of the particle size distribution along the centreline. The trends we observe are opposite for the measurement and prediction: While the experimentally determined standard deviation decreases, the standard deviation of the predicted particle size distributions increases. The first observation may again be taken as an indicator for predominant soot oxidation. The increase in standard deviation of the modelled particle size distributions, on the other hand, is difficult to rationalize. We conjecture that it is related to artificial diffusion effects in physical space, in particular, since the total number density on the centreline is over an order of magnitude smaller than in the enclosing flame wings.

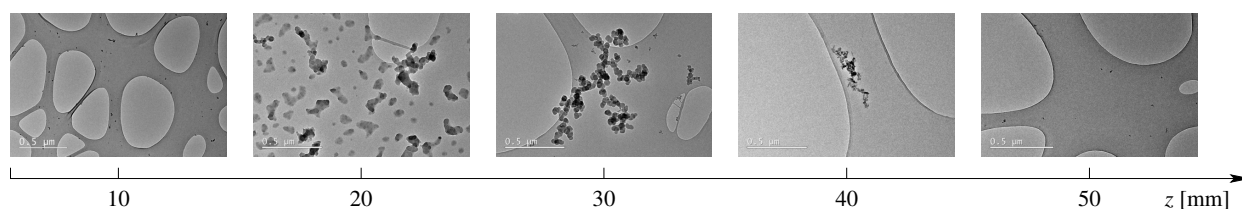


Figure 7: TEM images of thermophoretically sampled soot particles on the centreline of the flame.

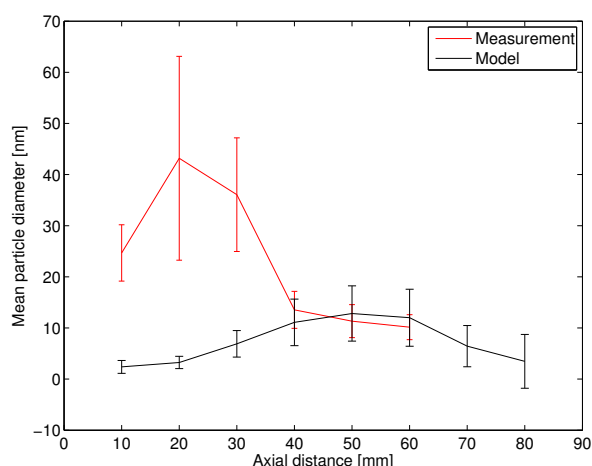


Figure 8: Mean primary particle size along the centreline of the burner. Here, the heights of the error bars indicate twice the standard deviation of the local particle size distribution.

Conclusions

We presented OH-LIF and ELS measurements used to characterize the chemical reactions and soot formation processes in a laminar diffusion flame. Our laser diagnostics were complemented by thermophoretic sampling of soot particles and TEM analysis. Both the novel experimental data and the measurements reported previously by Santoro et al. [3, 4] for a very similar flame configuration served as a basis for assessing the predictive capabilities of a comprehensive reacting flow/soot formation model. This model builds on the population balance equation and yields the primary soot particle size distribution at each spatial location in the domain.

Based on the predicted particle size distributions, we obtained model predictions of the ELS intensity distribution. Considering a signal-based comparison of experimental results and model predictions, we assessed the influence of polydispersity on the ELS signal, but found this to be almost negligible in the present configuration. This observation supports the common approach in which an estimate of mean particle size is obtained from experimental ELS signals by assuming a locally monodisperse particle population.

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