Summary on Discussion Session "Key Parameters for LII"

Discussion Leader: Stefan Will, University Erlangen, Germany

In continuation of similar session at previous LII workshops, the session aimed at reviewing the current status of knowledge on LII key parameters, identifying information gaps and giving directions for future work. Main parameters discussed include:

- Absorption Function $E(m)$
  As compared to early literature (Melton, frequent use of the refractive index m= 1.57-0.56i) further measurements (mainly by LII and extinction) have revealed a significantly higher value of E(m) than often used initially. The results of these studies may be summarized as:
  - "Mature" soot:
    - $E(m)$ @ 1064nm $\approx$ 0.4
    - E(532nm)/E(1064nm) $\approx$ 0.85 - 0.9
    - $E(m)$ @ 532nm $\approx$ 0.35
  - $E(m)$ decreases / $\text{ratio}_{532/1064}$ increases for "less mature" soot (higher H-content).
  - Considerable variation with temperature (graphitization)
- Thermal Accommodation Coefficient α
  Though the range of values used in the community has somewhat been narrowed down, there is still a large spread/uncertainty about this value.
  - A number of studies using LII have included aggregate shielding models to account for its effect on heat conduction. Potential uncertainties in these models and the application of various overall heat transfer result in fundamental uncertainties when deriving a "physical accommodation coefficient". LII studies suggest $\alpha \in$ [0.26; 0.38].
  - Direct measurements of gas-surface scattering are scarce and not available at temperatures relevant to LII. Extrapolating available data to higher temperatures results in considerably lower numbers, with $\alpha < 0.20$.
  - As for *E(m)*, also α-values seem to depend on soot maturity with α decreasing for more mature soot.
  - During the last years, molecular dynamics simulations have evolved as a valuable tool for the calculation of accommodation coefficients. Further MD-simulations and comparison with experiments under well-defined conditions (on isolated particles) are desired.
  - Further discussion has started if the provision of a certain value (as a function of maturity and other relevant parameters) is possible at all or if a probabilistic approach should be followed where it is assumed that the accommodation coefficient obeys some distribution.
- Density ρ / Heat Capacity c_s
  Obviously there is still a certain range of values used for these parameters (with a spread of the order of 10% each) resulting in some uncertainty in LII modelling. These effects are smaller than those from other parameters, neither are there dedicated approaches in sight that might improve the situation.
- Sublimation Coefficient β
  Experiments indicate that also the sublimation coefficient is subject to soot maturity. Further studies are needed to derive concise values.
- Influence of Particle Size
  Researchers are reminded that soot properties may depend on particle size. An example was given for evaporation properties.

- Concluding Discussion / Future Directions
  Apart from the points summarized above, the following general aspect has been given special consideration:
  Research during the last years has given clear indication that many key properties relevant for LII depend on the maturity of soot. For improved data interpretation, it seems necessary to take this aspect into account. Maturity is mainly related to hydrogen content (or, more general, to composition). As it is hardly possible to directly specify "maturity" in an LII experiment, research is needed to provide practical guidelines. Investigations in this context should focus on the analysis of composition of soot particles (from elemental analysis) for the various conditions found in flames. Practically, a relationship might be derived with a parameter that is comparatively easily accessible in experiments (such as the E(m)-ratio). This parameter might then be correlated to other parameters that also feature a dependence on "maturity" (such as accommodation coefficients).