Discussion session 1: Determination of key parameters for LII

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Main issues addressed

Main focus of the discussion was on few key parameters, which were selected based on the contributions sent from other researchers as well as based on our own considerations. The main discussion was about the absorption properties of soot, mainly through the absorption function E(m) and its dependence on conditions. Some discussion was also focused on the density and heat capacity of soot as function of temperature and maturity.

In the past, more than 15 years ago, optical properties were often expressed as complex refractive indices. Values from this literature have been nicely summarized in the paper by Bond and Bergström [T.C. Bond and R.W. Bergström, Aerosol Science and Technology 40, 27-67, 2006]. They discuss that soot refractive indices in the past showed large variations because the soot varied between the studies (various flame types and conditions) and that different techniques were used.

Mainly two techniques were used in the past to derive refractive indices; 1) reflectivity of compressed soot, and 2) scattering and absorption by suspended particles. Uncertainties are expected for both techniques and the paper says for example that" Refractive indices inferred from reflectance should be considered suspect" and "Both real and imaginary parts appear biased low if not corrected for void fraction or surface roughness".

E(m)-values in the literature based on refractive indices for studies in the past are often in the region 0.20-0.25. Recent in-situ investigations of mature soot indicate that E(m) is in the range 0.35-0.40. Although these derived values have uncertainties, they are considered to be more valid than the values in the range 0.20-0.25. (For example, the "famous" m=1.57-0.56i by Dalzell and Sarofim gives an E(m) of 0.260.) Several groups have continued to use older values for various reasons, for example that comparisons with old data is more straightforward. However, it seems relevant to establish these higher values of E(m) as better values of E(m) for mature soot. It also implies that soot volume fractions derived in flames in the past often are overestimated as a lower E(m)-value leads to a bias towards higher soot volume fractions. E(m) has been shown to vary as function of height above burner for soot, as they mature. This happens in some tens of milliseconds at temperatures of around 1800 K. These E(m)-measurements have been done in flames by measuring the initial flame temperature, heating the particles using specific pulse energy, and measure the heated particle temperature, under the assumption of constant product of density and heat capacity, i.e. $\rho \times c_p$. Recent search in the literature and extraction of information by H. Michelsen was presented on the meeting and her investigation indicated that the product of the density and heat capacity for soot was rather constant from flame temperatures to particle vaporization temperatures, and also that the product was rather constant as function of maturity (for variations in C/H-ratio). However, for low temperature, let´s say below 1500 K, there seems to be rather strong variation in the product $\rho \times c_p$.

Additional contributions to this session were the following:

H. Michelsen used LII fluence curves to instead of E(m) parametrize using two other variables; β for the wavelength dependence and ξ for the wavelength dependence and discussed her results in terms of maturity in a laminar sooting diffusion flame.

P. Desgroux discussed about the existence of “transparent nanoparticles”. The notation is somewhat misleading and could be a result of the limited possibility to make accurate extinction measurements **of very low soot volume fractions** in the past. With cavity-ringdown spectroscopy it is possible to measure those very low particle concentrations.