Impact of composition & morphology on soot optical properties

Swiss Federal Institute of Technology Zürich


G.A. Kelesidis[1], A. Bruun[1], M.R. Kholghy[1], L.S. Fan[2], S.E. Pratsinis[1]

[1] Particle Technology Laboratory, ETH Zürich, CH-8092 Zürich, Switzerland

[2] The Ohio State University, 43210 Ohio, U.S.A.

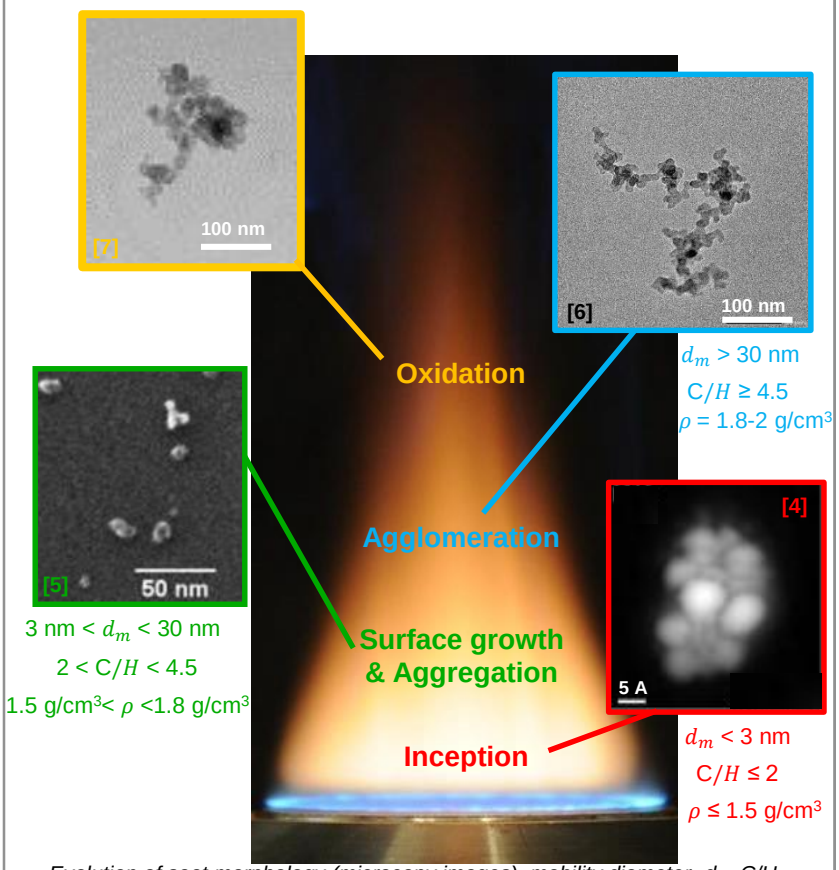
gkelesidis@ptl.mavt.ethz.ch

PTL www.ptl.ethz.ch

Motivation

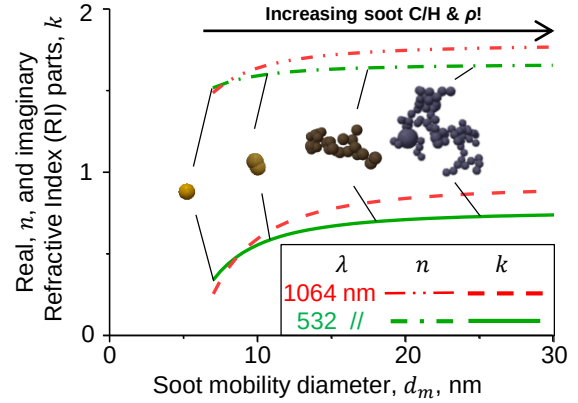
Soot optical properties are estimated by climate models using the Mie theory for spheres with a constant refractive index (*RI*) [1], neglecting the realistic soot composition and structure that vary between different combustion sources. This impedes the accurate estimation of the environmental impact of soot. Here, the Rayleigh-Debye-Gans (RDG) theory is revised using robust *RI* [2] and power laws [3] to estimate soot light absorption and scattering accounting for its detailed composition and agglomerate morphology.

Soot formation during ethylene combustion

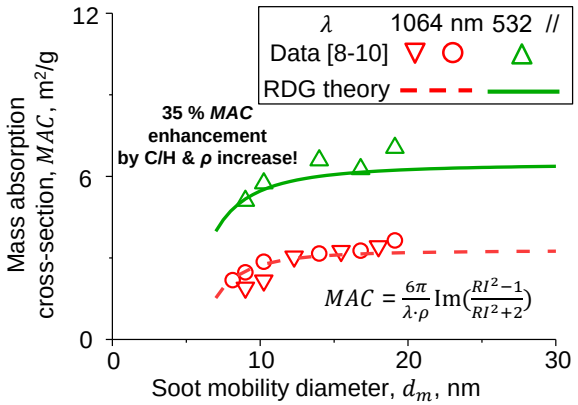


Evolution of soot morphology (microcopy images), mobility diameter, d_m, C/H and bulk density, ρ, during combustion in a premixed ethylene flame [6].

Soot *RI* [2] & light absorption dynamics

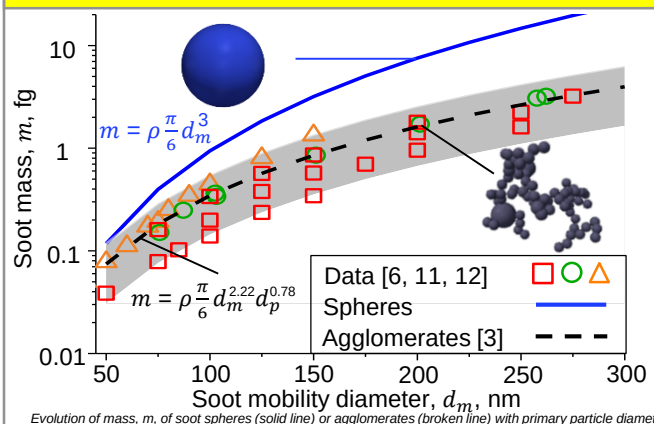


Real, n, and imaginary parts, k, of soot RI at wavelengths, λ = 532 and 1064 nm estimated as a function of d_m accounting for the evolving soot composition [2].

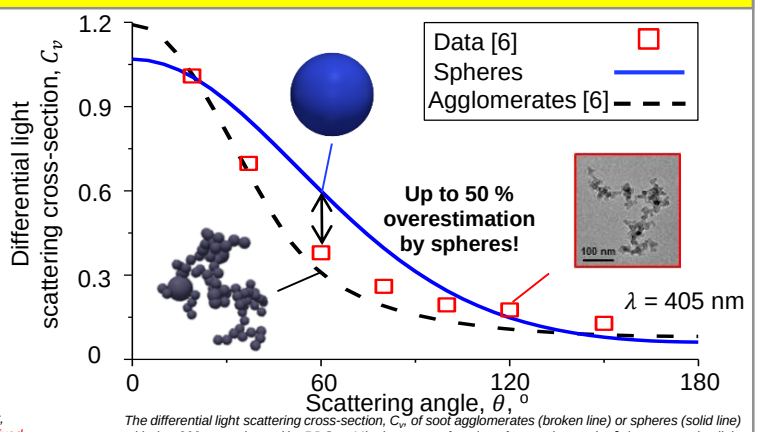


Soot mass absorption cross-section (MAC) estimated by RDG theory accounting for its evolving composition (lines) is compared to laser induced incandescence data from premixed ethylene [8; circles] and methane flames [9; triangles, 10; inverse triangles] at λ = 532 and 1064 nm.

Light scattering from soot nanoparticle agglomerates [6]



Evolution of mass, m, of soot spheres (solid line) or agglomerates (broken line) with primary particle diameter, d_p = 9-50 nm (shaded area) and ρ = 1.8 g/cm³ estimated as a function of their d_m is compared to data from premixed ethylene flames [6; squares], diesel car [11; circles] or aircraft engines [12; triangles].



The differential light scattering cross-section, C_v, of soot agglomerates (broken line) or spheres (solid line) with d_m =200 nm estimated by RDG or Mie theory as a function of scattering angle, θ, is compared to light scattering measurements in premixed ethylene flames [6; symbols] at λ = 405 nm.

References

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Conclusions

1. The RDG-derived soot light absorption increases up to 35 % due to the evolving soot composition and *RI*, in excellent agreement with data from premixed flames.
2. The soot mass-mobility relationship is described by a universal power law, assisting the accurate estimation of soot light scattering.
3. Climate models using the Mie theory for spheres overestimate soot mass up to an order of magnitude and its light scattering up to 50 %.
4. The RDG theory revised here to account for the realistic soot morphology and composition can be used to estimate accurately the climate impact of soot emissions from different combustion sources.