# Optical and morphological characterization of "miniCAST 5201 BC"-soot

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## Motivation

- Black Carbon (BC) and Brown Carbon (BrC) have a large impact on climate and cause adverse effects on human health.
- Carbonaceous particles are monitored with various types of instruments in ambient air or measured directly at emission sources.
- To ensure reliable and reproducible results, instruments should be calibrated with standardized and traceable calibration procedures.
- Thus, stable, reproducible and well-characterized soot aerosol generators are necessary, producing particles with well-defined physical characteristics.
- ➢ In this work, various set points of "miniCAST 5201 BC" burner have been further characterized focusing on optical and morphological properties of the particles.

## Methodology

- The miniCAST Model 5201 BC (Jing Ltd.)[1] was used as soot source and was operated at different conditions: a near-stoichiometric diffusion flame, three partially premixed fuel-lean flames and three fuel-rich diffusion flames.
- Soot aerosols were studied in terms of particle number size distribution (scanning mobility particle sizer SMPS), mass concentration (tapered element oscillating microbalance TEOM), nanostructure (Raman microspectroscopy and (high resolution) transmission electron microscopy TEM/HRTEM), composition (elemental and organic carbon EC/OC analysis) and optical properties (aethalometer AE33 and photoacoustic extinctiometer PAX at 870 nm).

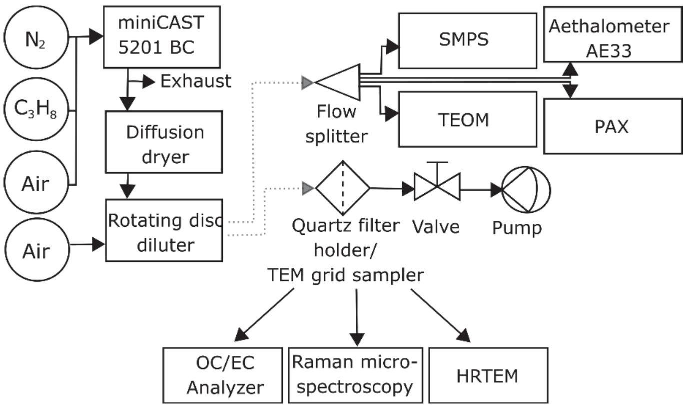
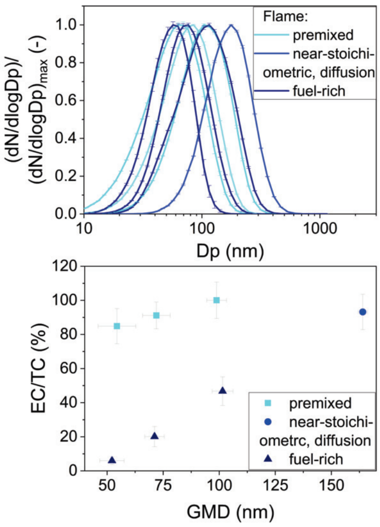



*Figure 1: Experimental setup for soot particle generation and characterization.*

## Particle size and composition




- The near stoichiometric diffusion flame generates particles with 160 nm geometric mean diameter GMD and high elemental carbon to total carbon EC/TC mass fraction (93%).
- Selected partially premixed near-stoichiometric fuel-lean flames (different gas compositions) generate particles with GMD 50 nm, 75 nm and 100 nm with high EC/TC mass fraction (85%, 92% and 100%).
- Selected fuel-rich flames (differ-ent fuel-to-air ratio) generate particles with 50 nm, 75 nm and 100 nm GMD and considerably lower EC/TC mass fractions (6%, 20% and 47%) than the fuel-lean flames.

*Figure 2: Normalized particle number mobility size distributions and EC/TC mass fractions of the generated particles.*

## Particle morphology

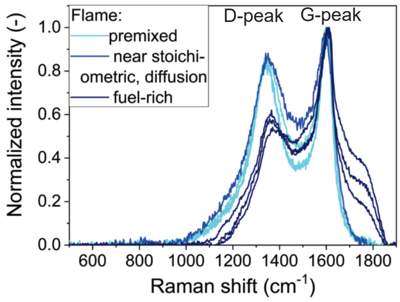



*Figure 3: Raman spectra of the soot samples.*

- As higher ratios of the Raman D-peak to G-peak indicate higher structural order for soot with small fringes[2,3] the "premixed" and "near-stoichiometric" soot is more ordered than the "fuel-rich" soot.
- Additional vibrations[4] of organic compounds appear in the Raman spectra of "fuel-rich" soot (increasing with decreasing EC/TC mass fraction).

- Primary particles of soot generated with the near-stoichiometric diffusion flame or with the partially premixed flames have a turbostratic, partially onion-like, structure.
- Primary particles of "fuel-rich" soot have a pronounced amorphous structure with some turbostratic regions.
- Raman and TEM results are in good agreement.

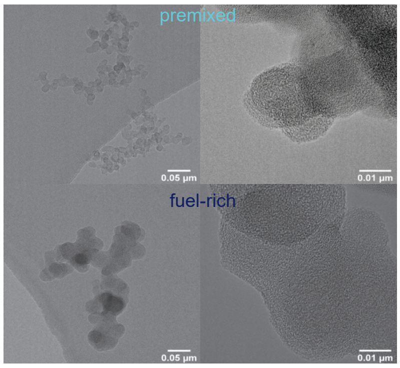



*Figure 4: TEM images of the selected soot samples: 100 nm particles generated with premixed and fuel-rich flames.*

## Optical properties of particles

- "Premixed" and "near-stoichiometric" soot:
  - Low wavelength dependence of absorption (Angstrom absorption exponent AAE < 1.2).
  - Low single scattering albedo (SSA < 0.01 to 0.12).
  - Particles mass absorption coefficients (MAC ≈ 4.3 to 3 $m^2/g$, from PAX-based absorption and TEOM mass), decreasing with decreasing particle size.
- "Fuel-rich" soot:
  - Higher AAE (1.7-3.4)
  - Higher SSA (≈ 0.2)
  - Lower MAC (≈ 0.25 to 2 $m^2/g$, indicating a much higher organic carbon content).

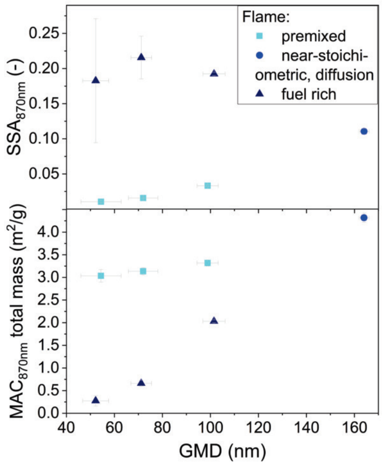



*Figure 5: SSA and MAC at 870 nm.*

## Summary and conclusion

- Stable and reproducible generation of soot with a wide range of properties with the miniCAST 5201 BC.
- Successful generation of soot particles with 50 nm to 160 nm mobility diameter, high EC/TC mass fraction (> 85%), high structural order and BC-like optical properties.
- Additionally soot material with the same size range but lower EC/TC mass fraction, lower structural order and rather BrC-like optical behavior (but not necessarily representative for ambient soot material) can be generated.
- ➢ BC-like soot from miniCAST 5201 BC can be used as surrogate for engine exhaust particles in order to calibrate engine exhaust CPCs or BC-monitoring instruments (e.g. absorption photometers).

## Literature

[1] Ess, M.N., and K. Vasilatou. 2019. *Aerosol Sci. Technol.* 53: 29–44.
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