Laboratory-based generation of particles simulating real ambient aerosols

Alejandro Keller, Daniel M. Kalbermatter, Kate Wolfer, Patrik Specht, Peter Steigmeier, Julian Resch, Markus Kalberer, Tobias Hammer & Konstantina Vasilatou

EMPIR

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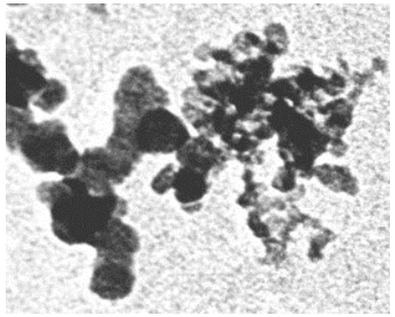
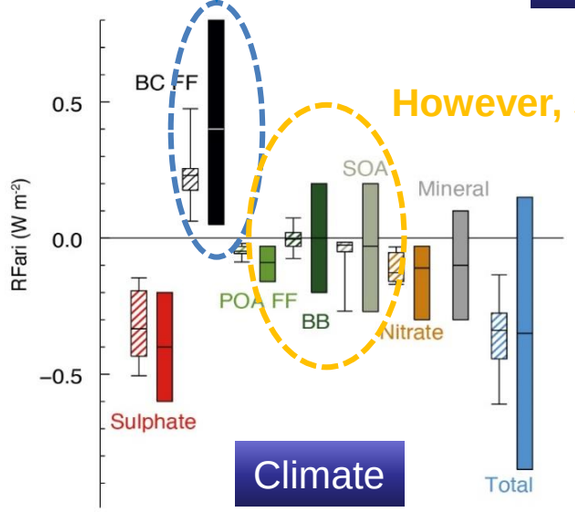
The EMPIR initiative is co-funded by the European Union's Horizon 2020 research and innovation programme and the EMPIR Participating States

Motivation



Soot: d_p~100 nm

Health effects



Climate

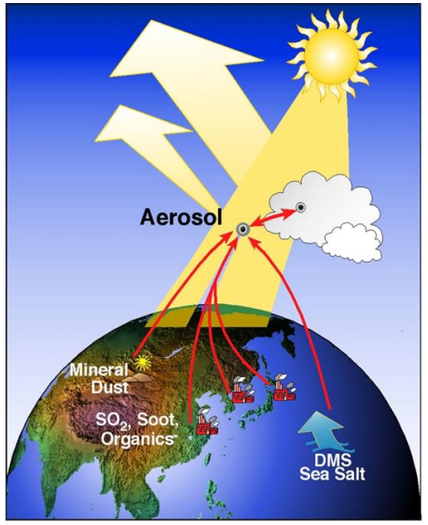
However, soot can be coated with primary or secondary organic material (SOA)

Atmosphere radiative forcing due to aerosol-radiation interactions (Rfari).
Source: IPCC 5th Assessment Report (AR5), 2013.

Coating ~~changes~~ determines the health impact

Is soot a trojan horse?

Coating changes radiative properties and affects climate relevant processes



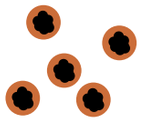
Generation of «fresh» and «aged» soot aerosols

Fresh soot particles

ozone, NO, OH
+ **organic vapours**

atmospheric ageing of soot
within a few hours or days

Aged soot particles



FIELD

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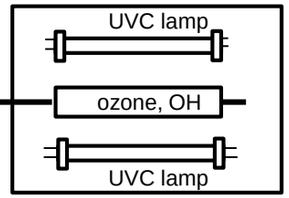
prototype miniCAST soot generator
Model 5201 BC

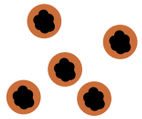
(Jing Ltd., Bern, Switzerland)

Oxidation flow reactor



organic vapours

Aged soot particles



LAB

Examples of oxidation flow reactors:

PAM
(Aerodyne Inc.)

Micro Smog Chamber

Volume: 150ml
Flow: 1 lpm
Residence time: ~10 Seconds
O_3: up to 100ppm (atmosphere < 60ppb)
Light: UVC (20W) and UVA (30W)

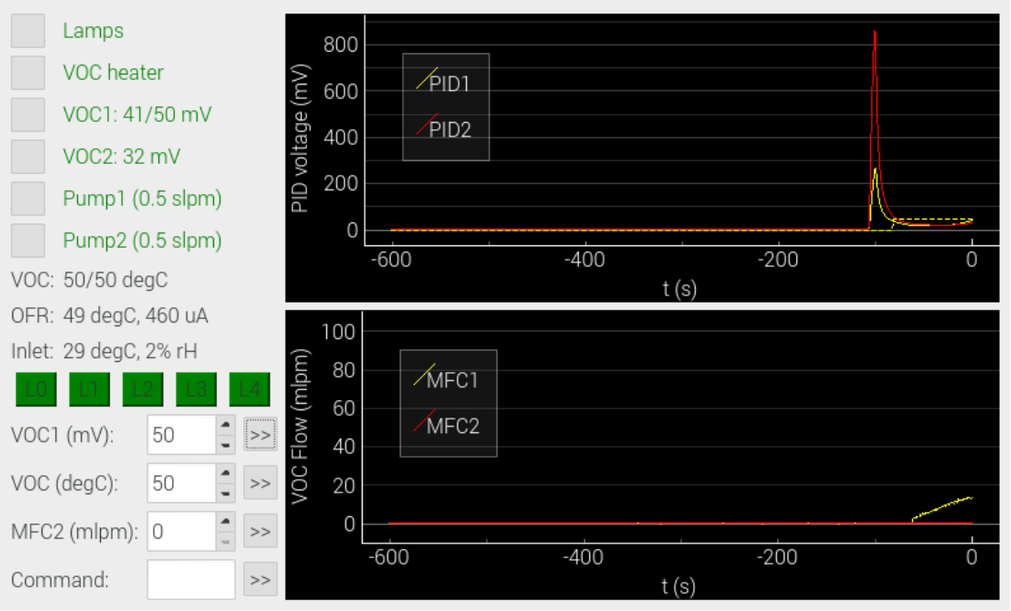
- **Unique:** Dimensioned for slightly diluted emissions (e.g. 1:10)
- No time resolved chemistry
- Oxidation degree can be adjusted through flow, length, or light intensity.

Keller & Burtscher, 2012, Aerosol Sci. 49 pp. 9-20

Ess et al. Journal of Aerosol Science (2021), doi.org/10.1016/j.jaerosci.2021.105820

Organic Coating Unit (OCU)

Controlled through GUI running on a microcomputer (Raspberry Pi or another device)



All-in-one instrument:

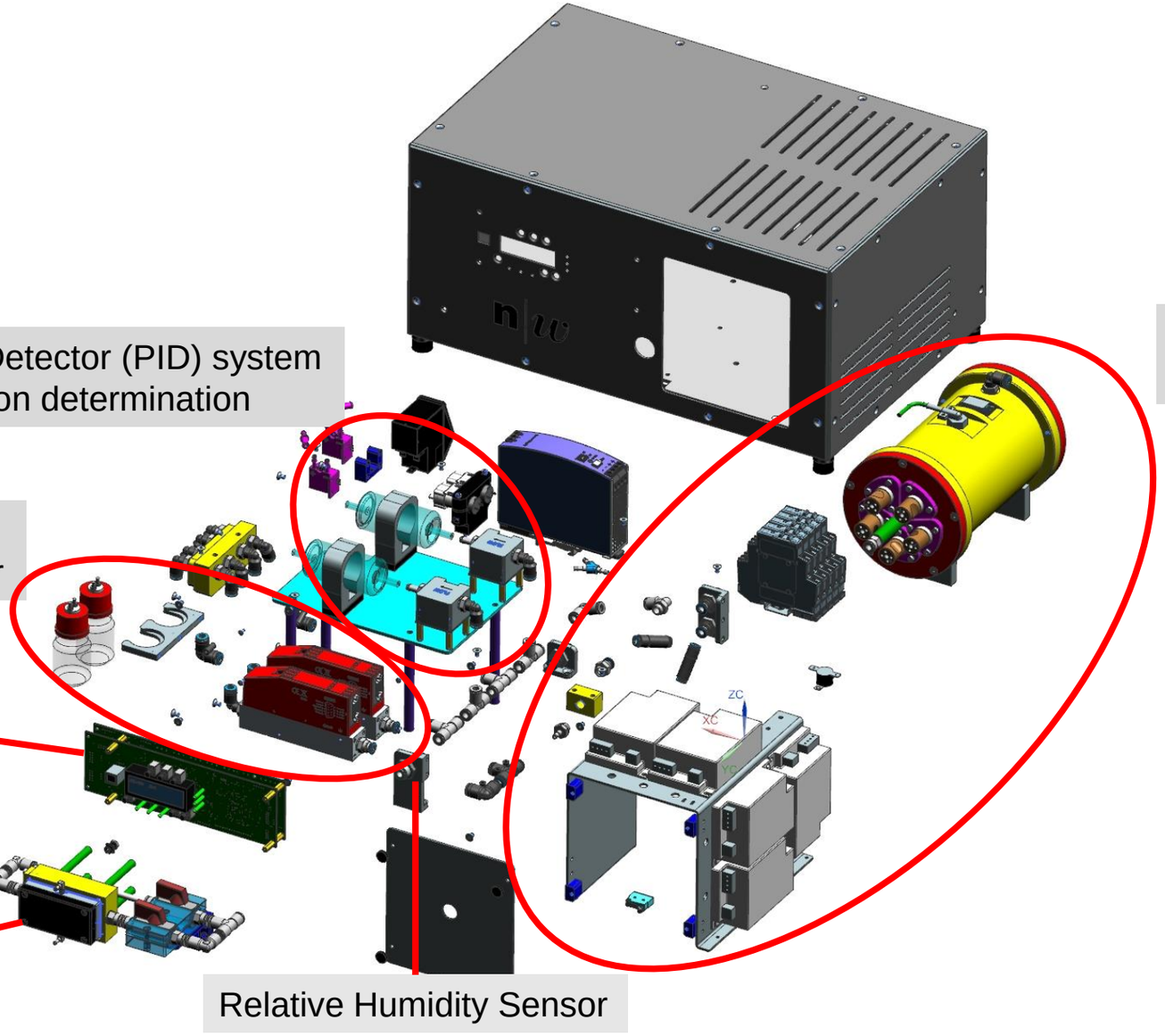
- Oxidation flow reactor
- VOC dosing system
- Aerosol humidifier
- User-friendly, automated, standardised

Log File:
Time
VOC concentration (i.e. 2x PID sensors)
VOC dosing temperature
MFC reading (i.e. dosing flow)
PID sensor flow
OFR Temperature
OFR UV intensity
Inlet rH and Temperature
Instrument and UV-lamps Status (systems that are on or off, etc)

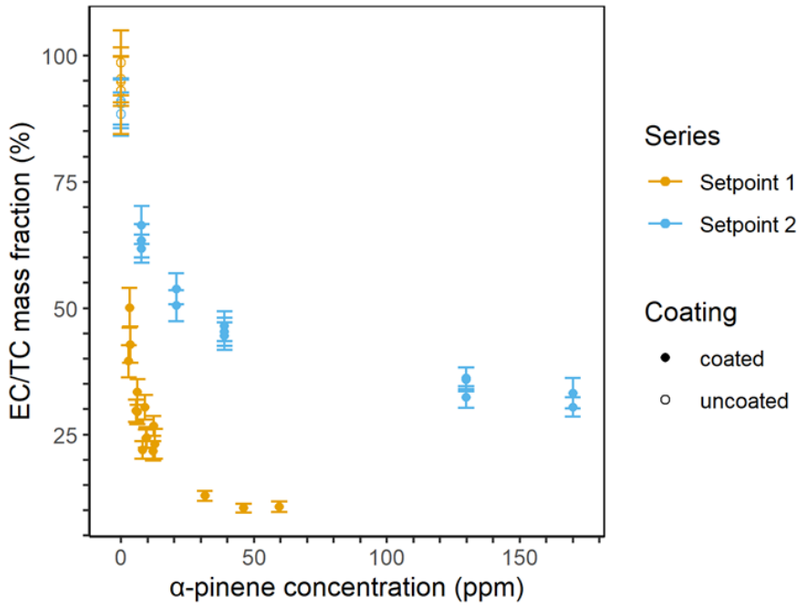
plus all relevant set points.

Keller et al., Aerosol Science and Technology 56:10, 947-958 (2022)
DOI: 10.1080/02786826.2022.2110448

Main Components



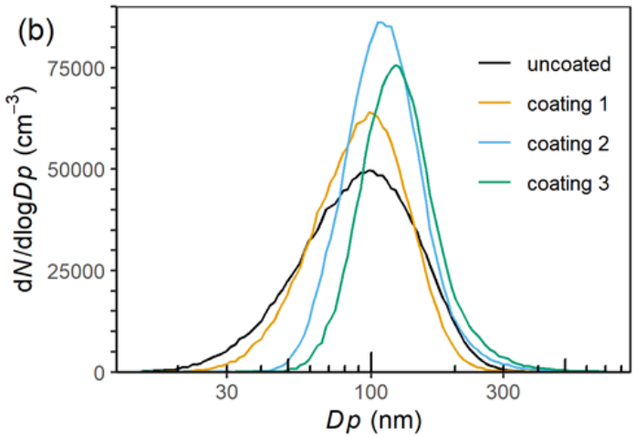
Aerosol properties

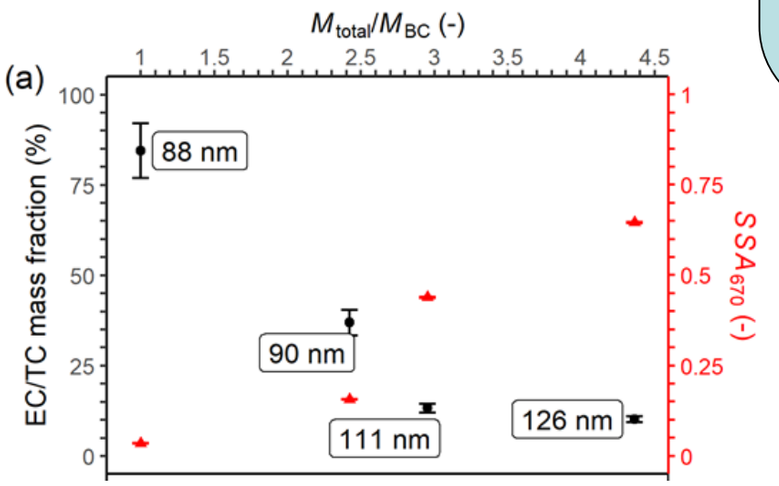


By varying miniCAST and OCU setpoints,
a wide range of aerosol properties can be attained

Select

according to application





Step-by-step tuning of

- particle size
- number concentration
- EC/OC mass fraction
- % SOA mass
- single scattering albedo

Chemical analysis of SOM with LC-MS

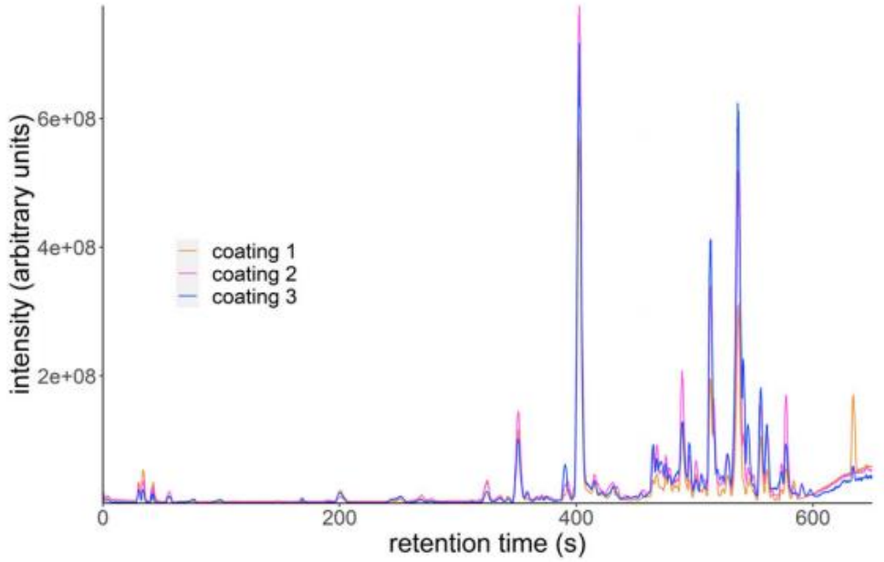


Figure 6. Base peak LC-MS chromatogram normalized per SOM mass collected and averaged for coating type.

Table 3. Summary of selected putatively annotated LC-MS features. CV: coefficient of variation (as ratio). Average numbers are given for formulae with multiple chromatographic features. Data are normalized to SOM mass values. n/a: not applicable. More detailed version of this table is given in Table S3.

Formula	Theoretical mass (m/z)	CV coating 1	CV coating 2	CV coating 3	Fold change 2/1	Fold change 3/2
$C_{10}H_{16}O_4$ (5 chromatographic features)	199.0976	0.45	0.48	0.27	1.43	0.98
$C_{10}H_{16}O_3$ (3 chromatographic features)	183.1027	0.52	0.53	0.22	1.65	0.85
$C_{10}H_{16}O_6$ (2 chromatographic features)	231.0874	0.53	0.36	0.20	0.82	0.95
$C_8H_{12}O_4$ (2 chromatographic features)	171.0663	0.33	0.27	0.12	0.98	0.73
$C_{10}H_{14}O_4$	197.0819	0.64	0.53	0.13	1.49	0.87
$C_9H_{14}O_3$	169.0870	1.33	1.16	0.12	1.74	2.36
$C_9H_{14}O_4$ (2 chromatographic features)	185.0819	0.47	0.29	0.14	1.24	0.88
$C_7H_{10}O_4$	157.0506	0.26	0.17	0.10	0.87	0.62
Average values	n/a	0.53	0.49	0.22	1.30	0.96

The composition compared well with other studies looking at the composition of a-pinene SOM confirming that the OCU generates SOM with a realistic overall chemical composition

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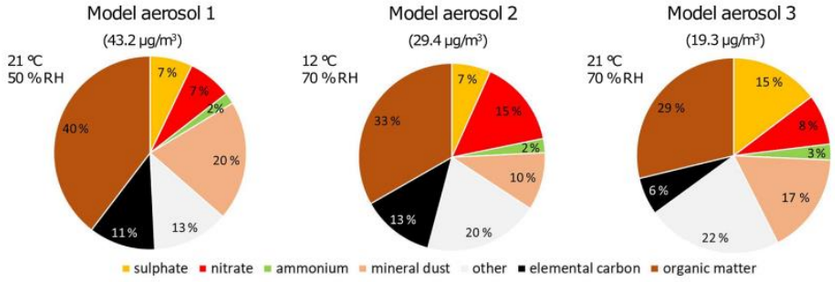
Generation of ambient-like particles in the laboratory



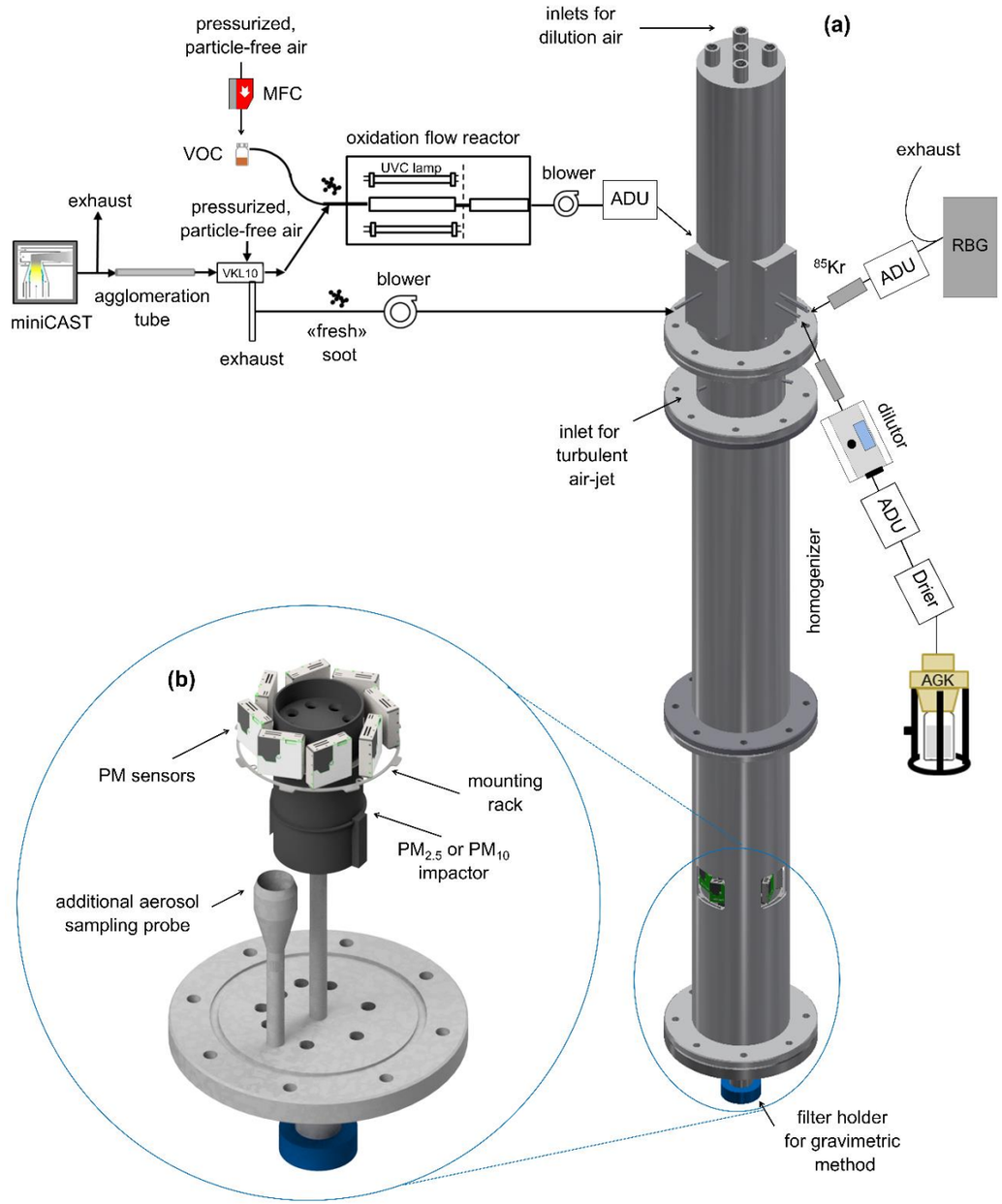
Large-scale facility for mixing

- fresh soot
- SOA
- inorganic matter
- mineral dust particles
- pollen (work in progress)

Advantages: Stable and reproducible aerosols
Known chemical composition

Applications

- Development of new aerosol instruments
- Calibration of Black Carbon monitoring instruments
- Calibration of PM monitors and low-cost sensors
- Machine learning of bioaerosol monitors
- In vitro toxicology



Horender et al., Atmos. Meas. Tech., 14, 1225–1238, 2021
Horender et al., Appl. Sci. 2021, 11(19), 9014

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Federal Institute of Metrology METAS

EMPIR AeroTox

AEROMET
Aerosol metrology for atmospheric science and air quality

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Thank you for your attention!