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Qualitative and Quantitative Characterization of Airport-related Ultrafine Particles using Liquid Chromatography – High-Resolution Mass Spectrometry (UHPLC/HRMS)

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We present the results from a chemical characterization study of ultrafine particles (UFP), collected nearby Frankfurt International Airport where particle size distribution measurements showed high number concentrations for particles with a diameter <50 nm. Aluminium filter samples were collected at an air quality monitoring station in a distance of 4 km to Frankfurt airport, using the 13-stage cascade impactor Nano-MOUDI (MSP Model-115). The chemical characterization of the ultrafine particles in the size range of 0.010-0.018 µm, 0.018-0.032 µm and 0.032-0.056 µm was accomplished by the development of an optimized filter extraction method. An UHPLC method for chromatographic separation of homologous series of hydrophobic and high molecular weight organic compounds, followed by heated electrospray ionization (ESI) and mass analysis using an Orbitrap high-resolution mass spectrometer was developed. Using a non-target screening, ~200 compounds were detected in the positive ionization mode after filtering, in order to ensure high quality of the obtained data. We determined the molecular formula of positively charged adducts ($[M+H]^+$; $[M+Na]^+$), and for each impaction stage we present molecular fingerprints (Molecular weight vs Retention time, Kroll-diagram, Van-Krevelen-diagram, Kendrick mass defect plot) in order to visualize the complex chemical composition. The negative ionization mode led only to the detection of a few compounds (<20) for which reason the particle characterization focuses on the positive ionization mode. We found that the majority of detected compounds belong to homologous series of two different kinds of organic esters, which are base stocks of aircraft lubrication oils. In reference to five different jet engine lubrication oils of various manufacturers, we identified the corresponding lubricant base stocks and their additives in the ultrafine particles by the use of matching retention time, exact mass and MS/MS fragmentation pattern of single organic molecules. As the relevance of the chemical composition of UFP regarding human health is depending on the mass contribution of each compound we strived for quantification of the jet engine oil compounds. This was achieved by standard addition of purchased original standards to the native sample extracts. Two amines serving as stabilizers, one organophosphate used as an anti-wear agent/metal deactivator and two ester base stocks were quantified. Quantification of the

two homologous ester series was carried out using one ester compound and cross-calibration. The quantitative determination is burdened by the uncertainty regarding sampling artefacts in the Nano-MOUDI. Therefore we characterized the cascade impactor in a lab experiment using the ester standard. Particle size distribution measurements conducted parallel to the filter sampling enables the determination of jet engine oil contribution to the UFP mass. Results indicate that aircraft emissions strongly influence the mass balance of 0.010-0.018 µm particles. This contribution decreases for bigger sized particles (0.018-0.056 µm) as presumably more sources get involved. The hereby-introduced method allows the qualitative and quantitative assignment of aircraft emissions towards the chemical composition and total mass of airport related ultrafine particles.