**Title:** Aerosol Single Particle Composition via STEM/EDS

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**1.0 Data Set Overview:**

These data files contain the percent by number of aerosol particle types collected at different flight levels on the C-130 aircraft and analyzed via Scanning Transmission Electron Microscopy Energy-dispersive X-ray Spectroscopy (STEM/EDS) during WE-CAN. Samples were collected via impaction in two dry size ranges as described below. Samples were collected mostly in ambient air and sometimes in cloud after droplet evaporation; samples in precipitating clouds or with ice were excluded. Since funding was limited, samples were analyzed from only a small selection of flights. Data are further presented and discussed in *Twohy et al.* [2021].

**2.0 Instrument Description:**

Aerosol particle samples were collected outside of clouds with a stainless steel Solid Diffuser Inlet based on the University of Hawaii SDI [*McNaughton et al.*, 2007; *Barry et al.*, 2021], as well as in clouds using a Counterflow Virtual Impactor (CVI) inlet [*Noone et al.*, 1988; *Twohy et al.*, 2003]. The CVI inlet and porous tube were composed of titanium and the sample lines were stainless steel. The CVI inlet was heated to ~50°C during cloud sampling in order to evaporate cloud droplets larger than 7-8 $\mu m$ diameter, and the sample stream heated to prevent condensation prior to measuring the associated water vapor with a tunable diode laser hygrometer. Particles from both inlets were collected with a two-stage impactor onto 200 mesh formvar-coated electron microscope grids in two dry diameter ranges of about 0.1-0.5 μm and 0.5-5 μm (assuming spherical particle densities of 1.5 g $cm^{-3}$ at typical sampling pressures of 600 mb). The elemental composition of selected samples was measured on a JEOL JEM-2100F 200 kV scanning transmission electron microscope with Oxford Max 80 Energy Dispersive Spectroscopy (EDS) system at Colorado State University, using a low background Beryllium sample holder.

**3.0 Data Collection and Processing:**

For each sample, the grid was scanned for representative sampling areas where particles were sufficiently far from the jet center to avoid overlap, but heavily loaded enough to minimize any potential artifacts. For samples with particles visibly volatile under the beam, groups of particles were analyzed

together to minimize energy input per unit area per time so major elements could still be detected. Particles were separated into categories based on spatial mapping of their detected elements and morphology as given in Table 1 and discussed in *Twohy et al.* [2021].

*Table 1. STEM-EDS Particle Classification Scheme*

| *Category* | *Characteristic signature* |
|---|---|
| *Mineral (crustal) dust or Ash* | Silicates (rich in Si, variable Na, Mg, Al, K, Ca, and Fe), carbonates (Mg and/or Ca with large C peak), phosphates (rare), usually non-spherical with irregular shapes |
| *Sulfur-based* | Round shape, primarily S, O, may be volatile under the electron beam. (Sulfuric acid, ammonium sulfate/bisulfate or MSA) |
| *Organic* | C above background and may contain O, K, N, S, Na also |
| *Soot* | C only plus characteristic chain aggregate morphology |
| *Metals* | Metals such as Al, Fe, Cr, Ti, Mn, Co, Zn, Cu, sometimes mixed with C |
| *Sea-spray Na* | NaCl with minor Mg, S, K, Ca, may also contain detectable C. Usually with crystalline structure |
| *Sea-spray high S* | Primarily Na with S>Mg by atomic weight, usually with K, Ca. May or may not contain detectable Cl and C |
| *Other Salt* | K, Ca, or Mg with minor Na relative to sea-spray, with Cl or S |
| *Mixed* | Combination of organics with other category types |

**Table 1 Notes.** Chemical and morphological features used to identify different types of particles via scanning transmission electron microscopy and energy-dispersive X-ray analysis.

**4.0 Data Format:**

There are two short csv data files, SingleParticleCompositionSmall.csv for the 0.1-0.5 micron diameter particles and SingleParticleCompositionLarge.csv for the >0.5 micron diameter particles. The column variables include:

**Flight**: flight number as used by the NCAR flight facility in WE-CAN, e.g., RF11 for Research Flight 11
**Date:** date in Day-Month-Year format for which sample was collected in UTC (not necessarily start date of flight)
**Sample:** sample number as used in WECAN
**Diameter:** diameter range in microns for dry spherical particles with densities of 1.5 g $cm^{-3}$ (at typical sampling pressures of 600 mb)
**Level**: GPS altitude in meters from the aircraft data system was used, rounded to nearest 10 m. If in-cloud, with "InCloud_" prior to altitude
**Start UTC**: start time that samples were collected in HH:MM:YY UTC
**End UTC:** end time that samples were collected in HH:MM:YY UTC
**N:** number of particles used in each sample to calculate composition fractions

**Remaining nine columns**: fractional composition; i.e., 0.375 means 37.5% of the particles analyzed had the composition named in column header (see Table 1).

**5.0 Data Remarks:**

Sodium-based sea spray includes both particles comprised of mostly NaCl (with other inorganic and organic sea-salt components), as well as those in the sea-spray "high S" category, which also have sodium but are enriched in sulfur and depleted in chlorine due to uptake and condensation of sulfur gases [*McInnes et al.*, 1994]. Sulfur-based particles, which were almost exclusively in the >0.1-0.5 micron diameter range, are also likely to have some organic components that cannot be detected by STEM/EDS above the substrate background, particularly if they are volatile. Most of the particles analyzed for WE-CAN were not obviously volatile under the beam.

**6.0 References:**


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