Readme File for Huebert Group C-130 Total Aerosol Sampler 16 June 2008

Title:

Aircraft C-130 Bulk Aerosol Mass of Anions and Cations from TAS (Huebert)

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1.0 Data Set Overview

This data was collected from the NCAR/NSF C-130 during the PASE program. It consists of samples collected using a Total Aerosol Sampler (TAS) and analyzed using ion chromatography after being shipped to our lab at the University of Hawaii. We report soluble chloride, nitrate, sulfate, oxalate, bromide, sodium, ammonium, potassium, magnesium, calcium, and nonseasalt sulfate. Each of these is accompanied by an uncertainty derived by propagating errors from the blanks, flowmeter, and analytical procedures.

Included in the data set are the start and stop times of each sample, as well as the mean altitude of the C-130 during each sampling interval. These altitudes are GPS values from the NCAR-RAF data system. More detail on the location of each leg and the conditions of each flight can be found in the C-130 Flight Reports and C-130 data in the PASE catalog (http://catalog.eol.ucar.edu/pase/).

The first reported samples are from the second research flight (RF02), flown on 10 August 2007 Kiribati time. (The takeoff time was just before midnight on 10 August UTC. All times and dates in the data file are UTC.) All sample names start with TRF## (TAS Research Flight and 2-digit flight number) and end with the time (HHMM) the sampling began. Missions were flown from Cassidy Airport, Kiribati. The last sample is from the last research flight, RF14.

2.0 Total Aerosol Sampler Description

The TAS sampler was located outside the fuselage on the left side of the C-130. It is designed so that every particle entering its tip can be extracted and analyzed. A separate filter/cone unit is inserted into the sampler (by reaching through an access door from inside the aircraft) for each sample collected. All particles entering TAS will be either collected on the filter or deposited to the inner walls of the cone. By separately extracting both the interior of the cone and the filter and dividing the mass of each analyte by the volume of air sampled, we derive a defendable ambient bulk concentration of each analyte. Since there is no inlet tube (except for the liner that we extract after exposure), there is no concern about inlet losses causing sampling artifacts. A sealing mechanism closed the sampler except during exposure, to prevent contamination of the filter/cone unit when we were not sampling.

The removable cones that line the diffuser are about 150 mm in length, with an inlet orifice of about 6 mm diameter and an exit of just over 74 mm diameter. The exit opening is configured to sit tightly against a 90 mm Teflon filter. The cones are coated with Teflon to minimize the collection of acidic gases like nitric acid. The external tip of the structure that holds the removable cones was sized to allow for isokinetic sampling at a range of C-130 airspeeds (roughly 100 - 140 m/s). The nominal flowrate was 100 lpm, but this was manually adjusted in flight to achieve isokinetic sampling on each leg. Flows were measured by a TSI thermal mass flowmeter, which was calibrated against a volumetric standard before and after the field program. Most samples were exposed for between 20 and 60 minutes.

TAS cones were extracted by revolving for 15 minutes with 30 ml of DI water. All Teflon filters were pre-washed in ethanol and DI water prior to the program to reduce nitrate and sodium blanks. After exposure each filter was placed in a microclean polyethylene bag and shipped (on the weekly commercial flight) to the University of Hawaii for analysis. The filters were extracted using 1 ml of ethanol (to wet the filter) and 9 ml of deionized water, in an ultrasonic bath. All cone and filter extracts were analyzed by ion chromatography as soon as possible.

The extracts of cones and filters were analyzed by suppressed ion chromatography on two Dionex ICs (one for anions and one for cations), using procedures identical to those described by Huebert et al. (*JGR*, **103**, 16493-16510, 1998).

3.0 Data Collection and Processing

3.1 Description of sample collection

Teflon filters and cleaned cones were assembled the night before each flight in a designated lab area in the Ops Center at the Captain Cook Hotel. On each C-130 flight, all 12 sets of pre-loaded filter/cone units would be brought aboard. When ready for sampling, the operator (Rebecca Simpson, Rebecca Anderson, or Lee Mauldin) would load a filter/cone unit into TAS, lock it in place, and close the access door. When a sampling leg began, the inlet closure valve and a rear valve (to the flowmeter and pump) would quickly be opened to start flow through the sampler. Over a period of about a minute, the operator would adjust valves to achieve isokinetic flow. Flow would continue to the end of that sampling leg, at which time the valves were closed as

nearly simultaneously as possible. This filter/cone unit would then be replaced by one for the next sample. The units were always changed with gloved hands and stored in sealed containers.

3.2 Description of derived parameters and processing techniques used

Mass flow from the Kurz mass flow meter for each sample was recorded on both the RAF data system and our own personal computer. From these recorded values, sample volumes were calculated. Each flowmeter was calibrated prior to and after the program. Uncertainties in the flows were estimated at 5%.

3.3 Description of quality control procedures

During each flight one field blank was exposed. This was a filter/cone unit just like the others, which was mounted in the TAS and exposed for just 10 seconds. Thus, its handling and history were identical to the actual samples. The analyte for that flight's blank filter was subtracted from each of the filters (or cones for the cone blank) on that flight. Uncertainties were derived by propagating the errors from the flowmeters (5%), instrument detection limit, the entire project blank variability (so they are generous for any one flight), and the analytical uncertainty.

On most flights we identified some samples that look contaminated, with extremely high sodium, chloride, magnesium, and nitrate (but not in sea salt ratios). Since both the cone and filters were contaminated, it is clear the contamination did not occur during extraction (cones done on Xmas, filters done at UH) nor preparation. After much searching, we determined that cloud splatter was responsible for this contamination. It occurred only on legs with appreciable LWC at some point and was larger the more water we encountered. We do not know the surface from which the splatter occurred, but it was probably not the tip of the inlet: that was covered (and kept clean) when not sampling. It is more likely that the splatter was from either the TAS shroud or the fuselage, both of which spent more and more hours sitting in sea spray at the airport as the experiment progressed. The contamination became more pronounced later in the experiment. We eliminated all samples with significant cloud encounters and the remainder of the data set is free of dramatic outliers.

We also are not reporting methanesulfonate for TAS samples. The cone and filter extracts both include an interfering peak in the ion chromatogram that seriously overlaps MSA. We tried a variety of conditions and organic solvents in the eluent, but were unable to move the peaks apart enough to quantify MSA. Fortunately, this interferent was not found on the MOI aluminum substrates, so we do have MSA size distributions in that data set.

We also found some contaminated blanks, each of which had been exposed for 10-15 sec in TAS. Those were also removed from the data set. In view of the fact that we were preparing and extracting sampling media in a fan-filled building no more than 30 meters from a windy coastline, we are pleased that the remaining data is as good as it appears to be. Twice the project-wide standard deviation of the remaining blanks was used as the criterion for significance of above-blank analyte.

4.0 Data Format

The file structure is an Excel file.

The data is in 31 columns with 102 rows. The first row is a reminded of the units, while the second row is a listing of the tabulated parameters. All concentrations and uncertainties are reported as micrograms of analyte per standard cubic meter of air, $\mu g/sm^3$. A blank row separates each flight from the next. All other rows contain the data from a single airborne sample. No missing data indicators were needed.

Note that we chose NOT to use "less than" symbols for values that were below the detection limit. Rather, each apparent analytical value is tabulated alongside its uncertainty. The only exception is a few slightly negative values (due to blank subtraction from lightly loaded filters) which were set to zero. In some samples there was not enough analyte to exceed the blank variability and other sources of uncertainty, so the uncertainty is larger than the value. Tabulating the data this way puts the responsibility on the data user to avoid interpreting values that are below the detection limit.

We elected to use this approach for two reasons: when computing average values it is always a challenge to know how to treat "less than" values. By leaving the apparent value in, that gives a slightly more informed value to use for averages than half the detection limit. Furthermore, since we used the variability of blanks throughout the whole program as the basis of our uncertainty calculations, we believe the actual detection limit is better than what we cite.

The columns are:

- 1. Flight Number
- 2. Start Time of the sample, as HH:MM:SS. All times and dates are UTC.
- 3. End Time of the sample, as HH:MM:SS. Note that several samples were turned off temporarily (for low altitude turns), so there is an intermediate off and on which is listed under "Comments."
- 4. Start Date and Time of the sample, as YYYYMMDDHHMMSS. All times and dates are UTC.
- 5. End Date and Time of the sample, as YYYYMMDDHHMMSS. Note that several samples were turned off temporarily (for low altitude turns), so there is an intermediate off and on which is listed under "Comments."
- 6. The UH sample number: "T" (for TAS), Flight Number (RF02) and approximate start time as HHMM. In the files at UH this would also include the individual TAS cone number, which has been removed here.
- 7. G Alt: The GPS altitude at the beginning of this sample, in meters above sea level (ASL). In some cases, a single sample may have integrated over several attitudes. The plane had usually

- stabilized its altitude by the time our sample flow began. Note that these altitudes are provided as a guide only, and serious use of position data should be accompanied by looking at the detailed flight data in the C-130 files, which we cannot reproduce here.
- 8. Cl: Chloride ion concentration. The units are micrograms of chloride per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 9.Cl-Unc: the propagated uncertainty in chloride concentration
- 10. SO4: Sulfate ion concentration. The units are micrograms of sulfate per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 11.SO4-Unc: the propagated uncertainty in sulfate concentration
- 12. Oxalate: Oxalate ion concentration. The units are micrograms of oxalate per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 13.Oxal-Unc: the propagated uncertainty in oxalate concentration
- 14. Br: Bromine ion concentration. The units are micrograms of bromine per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 15.Br-Unc: the propagated uncertainty in bromine concentration
- 16. NO3: Nitrate ion concentration. The units are micrograms of nitrate per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 17. NO3-Unc: the propagated uncertainty in nitrate concentration
- 18. Na: Sodium ion concentration. The units are micrograms of sodium per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 19.Na-Unc: the propagated uncertainty in sodium concentration
- 20. NH4: Ammonium ion concentration. The units are micrograms of ammonium per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 21.NH4-Unc: the propagated uncertainty in ammonium concentration
- 22. K: Potassium ion concentration. The units are micrograms of potassium per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 23.K-Unc: the propagated uncertainty in potassium concentration
- 24. Mg: Magnesium ion concentration. The units are micrograms of magnesium per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.

- 25.Mg-Unc: the propagated uncertainty in magnesium concentration
- 26. Ca: Calcium ion concentration. The units are micrograms of soluble calcium per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 27.Ca-Unc: the propagated uncertainty in calcium concentration
- 28. NSS: Non-seasalt sulfate ion concentration, derived using sodium to correct for sea salt. The units are micrograms of sulfate per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 29.NSS-Unc: the propagated uncertainty in non-seasalt sulfate concentration
- 30. ICSum: The sum of all mass concentrations for ions analyzed by IC. Note that this will certainly be smaller than the total ambient mass concentration, due to the exclusion of organics, soot, and insoluble minerals. The units are micrograms of carbon per standard cubic meter of air. Standard conditions are 1 atmosphere (1013 mbar) and 298 degrees K.
- 31. Comments.

This is Version 1.0 of the Huebert group TAS data.

5.0 Data Remarks

The TAS data should be the most accurate (although perhaps not the most precise) measure of bulk anion and cation concentrations from the C-130. Since it eliminates any concern about modification of the ambient concentrations of any size particles by inlets, it should be free of biases either due to inlet losses or enhancement. The only concern is that it operated isokinetically, which we assured within a few percent throughout each sample. However, since each concentration is reached by extracting both a cone and a filter and subtracting a blank from each, the TAS data may well have lower precision than devices which analyze only a single filter, for instance.

Two types of artifacts are of concern, both related to semivolatile species. If we collected ammonium nitrate aerosol, for example, there is a chance that some of the NH₄NO₃ would evaporate to nitric acid and ammonia after collection on the filter, thereby causing an underestimate of ammonium and nitrate aerosol. We think this is unlikely to be significant here, since virtually all of our MOUDI samples showed nitrate to be on coarse particles and ammonium to be on fine ones. Ammonium nitrate is a secondary aerosol that is usually in the accumulation mode.

The other possible artifact is a positive one, due to the collection of acid gases on the filter or on previously-collected particles. Since we used Teflon filters and Teflon-coated cones, we do not

think that the sampling medium collected acid gases. It is possible, however, that alkaline dust on a filter could have collected either SO_2 or nitric acid. Since sulfate was rarely on the same size as calcium, we doubt that SO_2 was collected, but we cannot rule out the possibility that nitric acid had been adsorbed onto collected dust. It seems likely that this would have gone to completion in the atmosphere rather than on a filter, but we have no way of disproving the hypothesis that some observed nitrate was derived from nitric acid vapor that reacted on the filter with dust particles.

Software compatibility

The file FnlTasBh16June08.xls is a Microsoft 97-2003 Excel spreadsheet. It should import easily into spreadsheets or other programs.