**Readme File** for Huebert Group C-130 Micro-Orifice Impactor (MOI) Anions and Cations, (First version prepared on15 September 2008)

# ReadMe File, Version 2, Modified on 16 Sept 2008

# Title: Aircraft C-130 MOI sized Anions and Cations (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 high-flow micro-orifice impactors (MOI) built by MSP Corp (Model 131), with the upper stages modified for straight-in flow. This impactor has a higher flow rate (100 lpm) than the typical MOUDI impactor, and distributes particles across 6 stages and a backup filter. The nominal 50% cutpoints of the stages were 10, 5, 1.4, 0.77, 0.44, and 0.26 µm. Analyses of substrates and filters were done by ion chromatography of aqueous extracts.

We present our MOI data in ambient concentrations that have been corrected to the best of our ability for blanks and LTI enhancement. There was no need to correct for particle bounce due to the assumed properties of the marine aerosol being sampled (i.e. sticky wet particles vs. bouncy dry dust). This data set comes with uncertainties that include flow rates, blank corrections, and analytical uncertainties, so you can constrain the range of ion ratios in large and small particles defendably. (In fact, the ratios are even better, since the 5% flow uncertainty drops out.) However, these uncertainties do not include the potential distortions of the distributions during sampling.

We would be remiss if we didn't mention the potential for gas-phase artifacts. For  $NO_3^-$  there is the potential for collection of  $HNO_3$  on previously-collected alkaline particles or evaporation of  $NH_4NO_3$ . For  $NH_4^+$  there is the possibility that  $NH_3$  vapor reacted with  $H_2SO_4$  on the filter or that  $NH_4NO_3$  evaporated. For  $SO_4^-$  there is the potential that  $SO_2$  reacted on the filter with alkaline particles to produce NSS. However, impactors tend to reduce condensation artifacts relative to filters, since the gases don't touch the deposited particles much. Furthermore, our relatively short sampling times reduce the potential for evaporative artifacts, since they happen when vapors in equilibrium with particles disappear during extended sampling. Also, we didn't have much NH<sub>4</sub>NO<sub>3</sub> to evaporate, since most of the NO<sub>3</sub><sup>-</sup> was in a non-volatile form on big particles with Ca<sup>++</sup>. We don't believe gas phase artifacts are a major source of error in this data set.

The data set is in the form of an Excel spreadsheet that includes the sample name, the UTC (Greenwich) date of the sample start, the UTC start and stop times, GPS altitude (which may not be reliable in some cases), corrected concentrations of the ions in each size range (in nanograms of analyte per standard cubic meter of air: 1013 mbar and 298K), and the uncertainty of each value. Each sample includes 7 lines of concentrations and uncertainties, for the 6 stages and the backup filter. The uncertainties were derived by propagating errors from the blanks, flowmeters, and analytical procedures. More detail on the location of each sample and the conditions of each flight can be found in the C-130 Flight Reports and C-130 data for PASE.

The first reported samples are from the second research flight (RF02), flown on 2 August 2007. All research flights have a sample name starting with M for MOI, then RF and were flown from Cassidy Airport, Christmas Island, Kiribas. There are no samples for the first research flight because a leak and pump control problems introduced unresolvable uncertainties for that flight.

It is important to keep in mind what you can and cannot do with this data. You can use the data to look at ratios of various ions in each size range. You can separately characterize the seasalt mode and the accumulation mode. However, above 1-3 $\mu$ m, the potential exists for plumbing losses, and though our sampling configuration was set up to minimize this effect, there is no doubt that a portion of large particles were not able to make every turn in the tubing.

For many samples these chemical size distributions were collected simultaneously with TAS samples, which give accurate (if noisy) bulk aerosol ion concentrations, free of inlet artifacts for any size. It is comforting to have a dumb (but defendable) bulk concentration measurement at times.

#### 2.0 Instrument Description

Air was conveyed into the aircraft by a port-side low-turbulence inlet (LTI) that was dedicated to this MOI. The efficiency of this inlet was a function of many factors, including airspeed and particle size. Generally, it enhanced particles in the 0.7 - 1.4  $\mu$ m range by 3%, in the 1.4 - 5  $\mu$ m range by roughly 26%, and in the 5 - 10  $\mu$ m range by about 50%. Size-dependent losses in the MOI plumbing, which offset these to a (variable) degree, are discussed below. Inside the fuselage, the flow passed through a 3.5 cm ID metal Y section and about 1 meter of 1.9 cm ID conductive silicone tubing to the entrance of the MOI. The other branch of the Y went to a TSI model 3321 Aerodynamic Particle Sizer (APS), so both data sets were modified identically by the LTI.

Aluminum foil substrates were used in each impactor stage, and 90 mm, 1 µm pore-size Gelman Zefluor Teflon filters were used as the backup stage. The Al substrates were punched from foil at

UH. Both filters and substrates were washed to reduce the variability of their blanks.

The MOI contained a variable-speed DC pump in a feedback loop with a thermal mass flowmeter and P and T sensors, so that it maintained the volumetric flow at 100 lpm. We found that this system and the data-recording processor inside the MOI worked very well.

After exposure the stacks were unloaded in a makeshift lab (which in retrospect should have included a clean glove box). Each substrate and filter was placed in a microclean polyethylene bag and packed for shipping to Honolulu on a weekly flight from Christmas Island to Oahu. In the UH lab, the samples were extracted using 1 ml of ethanol (to wet the filter) and 9 ml of weak acid solution (10<sup>-5</sup> M trifluoroacetic acid) in an ultrasonic bath. Each substrate was extracted with 10 ml of the weak acid solution, but with manual agitation rather than ultrasound. The weak acid prevented the loss of ammonium ion, but it probably increased the dissolution of carbonates (and Ca?) relative to DI water. All filter and substrate extracts were analyzed by ion chromatography as soon after a flight as possible, which in most cases meant a few days to a few weeks after a flight to allow for shipping time to our lab in Honolulu.

The extracts 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 data collection

Stacks were loaded with substrates and filters the night before each flight. Just prior to a flight twelve stacks would be carried aboard the C-130 and one would be loaded into the MOI sampler. When ready for sampling, the operator (Steve Howell) would tell the control computer to begin sampling. This would start the MOI pump and open a valve behind the stack, to start flow through that stack. Flow would continue to the end of that sampling leg, which was usually between 20 and 70 minutes, at which time the valve was closed.

Because we needed to collect material over tens of minutes, most samples corresponded to level legs, with virtually no sampling during ascents and descents. The exception is that on a few legs we had to change altitude (usually to avoid clouds), during which we continued sampling. A few samples had to be shut off briefly due to rain, so those samples have more than one start and stop time.

The filters and substrates from each flight were unloaded from their holders as soon as possible after each flight. Substrate and filter holders were all washed with DI prior to loading the media for the next flight.

#### 3.2 Description of derived parameters and processing techniques used

Flow, temperature, and pressure for the MOI were logged by its dedicated processor and then downloaded to a personal computer. Uncertainties in the flows are estimated at 3-5%. Relative humidity was also measured in the MOI, to estimate growth or shrinkage relative to ambient RH.

Concentrations were derived by first subtracting the blank analyte from that on a substrate or filter. The above-blank analyte in nanograms was then divided by the volume of air sampled (in standard cubic meters at 298K and 1 atmosphere) to get ng X/sm<sup>3</sup>. The uncertainties were derived as:

 $\lambda(X) = SQRT\{ (0.05^{*}[X])^{2} + (2^{*}\sigma_{X}/V)^{2} + (DL_{x}/V)^{2} \}$ 

where  $\lambda(X)$  is the uncertainty in the atmospheric concentration, [X], of substance X,  $\sigma_X$  is the standard deviation of X on blanks in nanograms,  $DL_X$  is the analytical detection limit of the IC for X expressed as ng X in a 10 ml extract, and V is the sampled air volume in standard cubic meters.

# We generated "corrected" data from the apparent data:

The LTI enhances the concentration of large particles relative to ambient concentrations. This enhancement depends on a number of factors, including the altitude (density) of the ambient air and the airspeed of the plane. LTI enhancement factors were calculated for each sample using pressure and mass flow data from the inlet in combination with a number of other parameters (i.e. assumed particle density of 1g/cm3). The MBL and FT enhancement values we used were roughly as follows:

	0.5 µm	1 µm	2.5 µm	5 µm	7 µm	10 µm
FT	1.01	1.03	1.06	1.24	1.9	2.8
MBL	1.01	1.02	1.03	1.14	1.5	2.0

Since the efficiency of the LTI for 5 to 10  $\mu$ m particles changes by more than a factor of two over the range, we selected an effective value for the purpose of correcting the apparent data (Column I) that assumed most of the mass would be on sizes closer to 5 than 10  $\mu$ m. This assumption will no doubt be better for some samples than others.

# 3.3 Description of quality control procedures

During each flight one stack was exposed as a field blank. This stack was handled just like the others and was mounted in the MOI, but it was exposed for only 10 seconds. Thus, its handling and history were identical to the actual samples. The mass of each analyte from the 6 substrates in a day's field blank stack were averaged and subtracted from the analyte on that days sample substrates. The same was true of the Teflon filter in the blank stack. Twice the standard deviation of a day's substrate blanks was used for the blank uncertainty (see above). For the Teflon filter blank variability, certain flights were removed due to an obviously contaminated blank. As in the equation above, uncertainties were derived by propagating the uncertainties from the analytical uncertainty and flowmeters (5% of the value), the instrument detection limit, and twice the blank variability, as a sum of squares.

#### 4.0 Data Format

The file is an Excel spreadsheet, prepared on PC with version Excel 2007, saved as an Excel 97-2003 spreadsheet for compatibility.

The columns are:

A. Sample name, as MRF##HHMM LJ, where ## is the flight number, HHMM is the UTC start time of the sample, L identifies it as a substrate sample and J is the stage of that stack. F is used instead of LJ for filter samples.

B. Date of the start of the sample, in UTC

C. Sample start time, UTC, as HHMMSS. Seconds were not recorded for the beginning of RF14.

D. Sample stop time, UTC, as HHMMSS. Seconds were not recorded for the beginning of RF14.

E. The nominal 50% cut size of the stage in  $\mu$ m aerodynamic diameter.

F. The geometric mean of sizes that should be collected by each stage, which we customarily use as the X-axis for plotting MOI distributions.

G. GPS altitude in meters above sea level, as recorded in the RAF data.

H. The corrected methane sulfonate concentration on each stage, in ng MS<sup>-</sup>/sm<sup>3</sup>.

I. The corrected chloride concentration on each stage, in ng Cl<sup>-</sup>/sm<sup>3</sup>.

J. The corrected sulfate concentration on each stage, in ng SO<sub>4</sub>-/sm<sup>3</sup>.

K. The corrected oxalate concentration on each stage, in ng Ox<sup>-</sup>/sm<sup>3</sup>.

L. The corrected bromide concentration on each stage, in ng Br<sup>-</sup>/sm<sup>3</sup>.

M. The corrected nitrate concentration on each stage, in ng NO<sub>3</sub><sup>-</sup>/sm<sup>3</sup>.

N. The corrected sodium concentration on each stage, in ng Na<sup>+</sup>/sm<sup>3</sup>.

O. The corrected ammonium concentration on each stage, in ng NH<sub>4</sub><sup>+</sup>/sm<sup>3</sup>.

P. The corrected potassium concentration on each stage, in ng K<sup>+</sup>/sm<sup>3</sup>.

Q. The corrected magnesium concentration on each stage, in ng Mg<sup>++</sup>/sm<sup>3</sup>.

R. The corrected soluble calcium concentration on each stage, in ng Ca<sup>++</sup>/sm<sup>3</sup>.

S. The corrected non-sea salt sulfate (NSS) concentration on each stage, in ng  $SO_4^{=}/sm^3$ . NSS was derived by subtracting the product of the seawater ratio of sulfate mass to sodium mass (0.251) and the observed sodium concentration from the observed sulfate concentration.

U. The uncertainty in the corrected methane sulfonate concentration on each stage, in ng MS<sup>-</sup>/sm<sup>3</sup>.

V. The uncertainty in the corrected chloride concentration on each stage, in ng Cl<sup>-</sup>/sm<sup>3</sup>.

W. The uncertainty in the corrected sulfate concentration on each stage, in ng SO<sub>4</sub>/sm<sup>3</sup>.

X. The uncertainty in the corrected oxalate concentration on each stage, in ng Ox<sup>-</sup>/sm<sup>3</sup>.

Y. The uncertainty in the corrected bromide concentration on each stage, in ng Br-/sm<sup>3</sup>.

Z. The uncertainty in the corrected nitrate concentration on each stage, in ng NO<sub>3</sub><sup>-</sup>/sm<sup>3</sup>.

AA. The uncertainty in the corrected sodium concentration on each stage, in ng Na<sup>+</sup>/sm<sup>3</sup>.

AB. The uncertainty in the corrected ammonium concentration on each stage, in ng NH<sub>4</sub><sup>+</sup>/sm<sup>3</sup>.

AC. The uncertainty in the corrected potassium concentration on each stage, in ng K<sup>+</sup>/sm<sup>3</sup>.

AD. The uncertainty in the corrected magnesium concentration on each stage, in ng Mg<sup>++</sup>/sm<sup>3</sup>.

AE. The uncertainty in the corrected soluble calcium concentration on each stage, in ng Ca<sup>++</sup>/sm<sup>3</sup>.

AF. The uncertainty in the corrected non-sea salt sulfate (NSS) concentration on each stage, in ng  $SO_4^{=}/sm^3$ .

#### Software compatibility

The file MOIHuebertSubmitOct02.xls is an Excel file which should open with most recent versions of Excel.