

TITLE: C-TOF-AMS ICE-L DATA ARCHIVE

AUTHORS: Dr. Shane Murphy, Prof. John H. Seinfeld
California Institute of Technology
1200 East California Blvd, M/C 210-41
Pasadena, CA 91125
Phone: (626) 395-4635
Fax: (626) 796-2591
E-MAIL: seinfeld@caltech.edu, shane.murphy@noaa.gov (or
techsmurph@gmail.com)

1.0 DATA SET OVERVIEW

This data set provides chemical composition data for non-refractory, sub-micron (vacuum aerodynamic diameter) aerosol gathered with an Aerodyne Compact Time of Flight Aerosol Mass Spectrometer. Air was sampled through a heated NCAR HIAPER Modular Inlet (HIMIL) during clear air and through Cynthia Twohey's counterflow virtual impactor (CVI) during cloud passes. The measurements were made during the Ice in Clouds Experiment - Layer Clouds (ICE-L) based out of Broomfield, CO on the C-130 aircraft from Nov.-Dec. 2007. Data is included for the following flights: RF01, RF02, RF03, RF04, RF05, RF06, RF07, RF08, RF09, RF10, RF11, and RF12.

2.0 INSTRUMENT DESCRIPTION

The Aerodyne Compact Time of Flight Aerosol Mass Spectrometer has been described previously for both ground-based (Drewnick et al., 2005) and airborne measurements (Murphy et al., 2009). During ICE-L the C-TOF-AMS was fitted with a constant pressure inlet to avoid changes in sizing and mass concentration with altitude (Bahreini, 2008). The instrument had a 3.5% chopper and ion extraction occurred at a rate of 60 kHz. The vaporizer of the instrument was set to ~550 degrees Celcius meaning that reported measurements of refractory species (Chl) do not represent

the full mass loading of that species but are an indicator of changes in mass loading. The mass loadings reported were calculated using the standard fragmentation table for Aerodyne AMS (Jimenez et al., 2003) except for slight modifications when measuring on the CVI to account for the switch from air to the pure nitrogen used as a carrier gas in the CVI. Detection limits for the instrument, calculated as three times the standard deviation of the noise for filtered air, are $<0.05 \mu\text{g m}^{-3}$ for all species measured, though, in practice, detection is limited by counting statistics at low aerosol loadings. One important issue concerning C-ToF-AMS data is the collection efficiency of particles within the instrument (Huffman et al., 2005). A collection efficiency (CE) of 1 was used for this data set. Typically a CE of roughly 0.5 is applied to ambient data collected with an Aerodyne C-TOF-AMS, but during ICE-L a CE of 1 gave the best agreement between the C-TOF-AMS mass loadings and the UHSAS volume loadings multiplied by an estimated bulk density of 1.6. Given that the UHSAS measures refractory components in addition to the non-refractory components measured by the C-TOF-AMS, one would expect the UHSAS derived mass to be equal to or greater than the C-TOF-AMS if a density of 1.6 is reasonable. Given that the C-TOF-AMS mass was already often equal to or greater than the UHSAS derived mass (with an assumed density of 1.6) with a CE of 1, this was chosen for the CE throughout the mission. However, given the lack of an exact way to determine the CE, it should be noted that C-TOF-AMS mass total loadings could be up to a factor of 2 low in worst-case time periods if the CE was changing. It is very important to note that even if the CE was wrong during certain and the absolute mass loadings are off, the relative masses of the different species measured should be correct.

3.0 DATA COLLECTION AND PROCESSING

Both clear air and cloud samples were analyzed using the

Squirrel ToF-AMS Analysis

Toolkit Version 1.44 data analysis package. Mass concentrations were calculated in the normal way for Aerodyne AMS systems, based on calibration with ammonium nitrate. as discussed above, a collection efficiency of 1. The masses reported when the C-TOF-AMS was pulling air from the NCAR CVI (Cynthia Twohy, Oregon State Univ.) have already been corrected for the enhancement in particle concentration that the CVI creates. The enhancement factors used for this correction are reported in the CVI data set for ICE-L. The data set that is being archived here does not include size-resolved data because, in general, the mass loadings during ICE-L were low enough that this size resolved data is quite noisy and requires long averaging periods (several minutes or more during most of the mission, unless loadings were higher than average). If you are interested in the size resolved data, we can provide it upon request. Requests should be sent to Shane Murphy at the e-mail addresses given at the top of this document.

4.0 DATA FORMAT

The accompanying data set file is a column delimited ASCII file. The columns are described below. All masses are in micrograms per cubic meter

Column Number	Column Name	Measurement
1	UTC	Time in seconds after
	midnight. Time stamps	are the end of the
	measurement period. In other	words the masses in that
	row are averaged from the	previous row's time

until the time given in that row

2	cvi_on1_off0	Flag, if set to 1 the C-ToF-AMS is pulling from the CVI, if set to 0 the C-ToF-AMS is pulling from the HIMIL inlet
3	TOTMASS	The total non-refractory mass measured by the C-TOF-AMS
4	ORG	The mass of non-refractory organic
5	SO4	The mass of non-refractory sulfate
6	NO3	The mass of non-refractory nitrate
7	NH4	The mass of non-refractory ammonium
8	CHL	The mass of non-refractory chloride
9	ORGMZ43	The non-refractory organic mass at m/z 43
10	ORGMZ44	The non-refractory organic mass at m/z 44 indicative of oxygenated organic mass
11	ORGMZ57	The non-refractory organic mass at m/z 57 indicative of hydrocarbon-like organic
12	ORGMZ60	The non-refractory organic mass at m/z 60 indicative of biomass

burning

13	MZ23	Non-quantitative
measure of mass at m/z 23		indicative of sodium
14	MZ39	Non-quantitative
measure of mass at m/z 39		indicative of potassium

The times are not a constant number of seconds apart because of slight changes in the time required for the instrument to write the data to file. However, data is typically reported every ~20 seconds.

5.0 DATA REMARKS

We ask all users of this data to contact Prof. John Seinfeld or Dr. Shane Murphy before publication of results involving this data.

6.0 REFERENCES

Bahreini, R., et al., "Design and operation of a pressure-controlled inlet for airborne sampling with an aerodynamic aerosol lens" *Aerosol Science and Technology*, 42 (6) 465- 471, 2008.

Drewnick, F., et al., "A new Time-of-Flight Aerosol Mass Spectrometer (ToF-AMS) - Instrument Description and First Field Deployment" *Aerosol Science and Technology*, 39:637-658, 2005.

Huffman, J. A., et al., "Design, modeling, optimization, and experimental tests of a particle beam width probe for the aerodyne aerosol mass spectrometer" *Aerosol Science and Technology*, 39, 1143- 1163, 2005.

Jimenez, J.L., et al., "Ambient Aerosol Sampling with an Aerosol Mass Spectrometer." *Journal of Geophysical Research - Atmospheres*, 108(D7), 8425, doi:10.1029/2001JD001213, 2003.

Murphy, S. M., et al., "Comprehensive simultaneous shipboard and airborne characterization of exhaust from a modern container ship at sea." *Environmental Science and Technology*, 43 (13), 4626-4640, 2009.