

ReadMe for NEAQS/ICARTT PALMS data files
Created 20041021 from itct readme file

PI: Daniel Murphy
NOAA Aeronomy Laboratory
325 Broadway, Boulder CO 80305
303-497-5640
Daniel.M.Murphy@noaa.gov

The PALMS exchange files are IGOR binary files with peak areas from the PALMS data as well as other data interpolated onto the time of each PALMS particle.

There are multiple sets of files: a set covers the entire mission and a duplicate set that separates each flight. There are no files for 20020429 because PALMS failed that day.

With a couple of exceptions, there are two subsets of files, one for positive ion mode and one for negative ion mode. Those exceptions are AllPALMSDateTime and AllPALMSPolarity, a set of all datetimes and a polarity flag for each particle (complete mission only).

***** IMPORTANT TIME FILES: *****

PosDateTimes, NegDateTimes: Date/time in Igor time format for the positive and negative mass spectra, respectively.

PosTimes, NegTimes: Time from midnight for that flight date in seconds. Will go past midnight for a single flight.

Pos, NegFlightCode: Long integers with the 8 digit date code: e.g. 20020715. Most useful for the entire mission files: you already know the date for the single flight files!

PosFlightCode2004, NegFlightCode2004: Except only the date in 2004: 715, ...

PosDCode,...: Also long integers with the date such as 20020715. The difference between this and FlightCode is that the DCode changes at UT midnight in the middle of the flight (it is the actual date) and FlightCode doesn't.

***** MASS SPECTRA FILES: *****

PosAreas1...PosAreas213 and negative counterparts:
The area of that peak in each positive or negative mass spectrum.
Units are fraction of the total signal for that spectrum.
In theory one could reconstruct a mass spectrum by reading in all the Areas files and taking the jth element of each file.

PosTotlon, NegTotlon: The total ion detector signal. For example, to find the absolute detector signal for NegAreas35, multiply it by NegTotlon.
Units are number of electrons*1000. Gain of the detector is VERY roughly

1000, so the number of ions in a mass spectrum is roughly $\text{TotIons}/1E6$.

Pos,NegAreasHMass: The total of all peaks above 213 (fraction).

Pos,NegAreasNoID: The total of all peaks with no mass ID (fraction).

Pos,NegAreasNonInt: The total of peaks at non-integer masses. For ITCT this is primarily 25.5 from doubly charged vanadium. The only other common doubly charged peak is 11.5 from doubly charged Na.

Pos,NegTotBackGnd: The total of background signal subtracted from the spectrum. (fraction). Zero or inconsequential throughout ITCT.

Helpful hints on important peaks to look at are in an accompanying file.

***** OTHER PALMS FILES: *****

Each has a Pos... and Neg... version.

ScatHt: A rough measure of the particle size.

The amount of light scattered by that particle in the trigger laser (V).

AeroDiam: The aerodynamic diameter (of the particles that went through both beams)

AeroDiam1p7: Aerodiam converted to geometric using a density of 1.7 g cm⁻³ assuming spherical particles.

CatPos and CatNeg: Results of a cluster analysis on the spectra. See section below.

... less useful to outsiders...

Confidence: A subjective confidence applied to the quality of a mass spectrum:

5: Minor problems...

8: Result of an automated analysis...

10: Great

Index: Index of the particle on that day - this is the jth particle we tried to zap.

JouleMtr: A measure of the excimer laser power on that shot (V).

MScaleA0, MScaleB0: The coefficients in fitting the time to mass conversion in the time of flight mass spectrum: $\text{mass} = a + b \text{SQRT}(\text{time})$. (time in us).

A very few spectra have more than one segment to the mass scale, if so, this is the first (low mass) segment.

MScaleSigs0: The variance (or sd?) of the peak positions from integers. Lower values indicate a better mass fit. Higher values are usually associated with wide peaks from mineral or salt particle.

ND: The neutral density filter in the excimer beam (transmitted fraction).

1.0 is no filter. This is another way of looking at the excimer laser power (besides JouleMtr).

NumPk: The number of peaks in the mass spectrum.

ScatW: The full width half max of the scatter light signal (us).

Seconds1999: Time since the beginning of 1999 (seconds).

... even less useful to outsiders...

ScatMaxSub: The subscript into the array where ScatHt was found.

TDay: Time of day since midnight on the day of the first flight (seconds).

***** PALMS CLUSTER ANALYSIS: *****

CatPos: results of cluster analysis on positive spectra.

CatNeg: results of cluster analysis on negative spectra.

...Vig: contains the dot product between each spectrum and its cluster.

A full description of our cluster analysis is in Murphy, Middlebrook and Warshawsky, "Cluster analysis of data from the Particle Analysis by Laser Mass Spectrometry (PALMS) instrument," Aer. Sci. Technol., in review in late 2002.

Basically, the data set are searched for the most similar spectra. These are averaged and then the next most similar spectra (or previous averages) are found and averaged... until there are a manageable number left. Some final combining is done manually with knowledge of the chemistry, etc.

The meanings of some of the more abundant clusters are in an accompanying file. The cluster analysis allows one to quickly ask questions like "where were there sea salt particles" without building up an elaborate set of criteria and without being quite so easily misled by double meanings for peaks (was that K from salt or biomass burning?). A warning on the cluster analysis is that it is a statistical technique and is not absolutely correct.

***** FILES OF OTHER DATA: *****

The PALMS data are on a different (and semirandom) time base. To facilitate comparing other data with ours, we are including files of most everything else that has exchange files. These data have been interpolated onto the time of each particle. Please let me (Dan Murphy) know if there are problems with using your data this way. THESE MAY NOT BE THE MOST CURRENT DATA.

The interpolation has two significant parameters. The first is a "gap size." That means the maximum spread in time between valid data point of a variable when it was still interpolated. For example, if a PALMS spectrum was between valid data points one second apart, it makes sense to interpolate, but not if there was an hour missing. For many variables (e.g. PTRMS), there are gaps between every valid data point, so one has to set the gap well above 1 second.

The other parameter is smoothing. The quality of comparison to the PALMS data is increased by smoothing. We've tried to strike a balance between level flight and plumes. Smoothing was with a symmetric boxcar; the number given is full width.

Some variables have been renamed slightly. All units are unchanged from their

exchange files.

Aircraft and chemical parameters:

NAME	GAP (s)	SMOOTH (s)	NOTES
DewPt	30	5	
dnPRT	30	3	
EqPO	30	5	
GPSAlt	30	3	
H2Omr	30	7	
Lat	30	3	
Lon	30	3	
PAIt	30	3	
PO	30	3	potential temperature
PR	30	3	
RAIt	30	3	radar altitude
RHW	30	5	relative humidity
TE	30	3	ambient temperature
WindDir	30	0	hard to smooth an angle
WindSpd	30	3	
WindVertSpd	30	21	
CO	15	5	
HNO3	15	7	
NO	15	7	
NO2	15	7	
NO3		200	3
NOY	15	5	
O3	15	3	
PTR-MS	200	21	low time rate
SO2	20	21	
Aerosol	15	7 for PM1, PM25, and Tot; 9 for Coarse	

(PTR-MS = Acetaldehyde, Acetone, Acetonitrile, Benzene, DMS, Isoprene, Methanol, Toluene, Xylene)

(Aerosol = NCoarse, NPM1, NPM25, NTot, SCoarse, SPM1, SPM25, STot, VCoarse, VPM1, VPM25, VTot)

***** MORE USEFUL STUFF: *****

Density: Air density in kg m⁻³. Useful for converting Hg and PILS data from per m³ to mass mixing ratio. This is the dry air density - the water partial pressure has been subtracted from the pressure.

WINDNS, WINDEW: Wind vector velocity (both sides of zero). The big reason for these is that they can be easily averaged. WindDir can't be just averaged or else angles of 5 and 355 average to 180, not 360.

TE_K: Temperature in Kelvin.