

Readme file for PALMS Single Particle data files.

There are two data files for each flight date: positive and negative ion spectra. These single particle data files include semi-processed data. Please consult with PALMS investigators for proper interpretation.

Each file includes an array of mass spectra plus ancillary data for each particle with a mass spectrum. The array of mass spectra includes unit mass resolution peak areas for each particle. The peaks are from m/z 0 to 239, plus a final element that is the sum of all peaks larger than m/z 239. In a zero-based array index the index number is the unit mass.

Peak areas are expressed as fractions of the total ion signal for that mass spectrum. Fractions are more consistent than absolute peak areas for particles that experience different laser ionization conditions because they happen to be in different parts of the excimer laser beam. Absolute areas can be recovered by multiplying the fractional peak areas by the TotalMCPSignal in the ancillary data.

Mass spectra are included that have reasonable ion intensity and mass resolution. During recent missions (ATom, SEAC4RS, and DC3) quality spectra were obtained for over 90% of the particles at which the excimer laser was fired. We believe misses are mostly random. In particular, the detection of small particles is optimized if the threshold for firing the excimer laser at a particle is set at a level that includes occasional noise triggers.

Mass spectra are included in these files only for sampling ambient air (not calibrations or background checks). Mass spectra from heavy clouds are excluded because of artifacts when cloud droplets and/or ice crystals hit the inlet.

To be useful, these data must usually be filtered for other conditions, including but not limited to consistent excimer laser power and excluding many thinner clouds.

Ancillary data for each particle:

FlightTDay (seconds): The UT time that the particle was sampled starting at midnight on the date of the flight. This time does not roll over at midnight but will continue to values larger than 24 hours.

DateTime (seconds): The time the particle was sampled in seconds since Jan 1, 1904 (a convention for Igor and some other languages). This is double precision.

Altitude, Latitude, Longitude (m, degrees): Aircraft position at the time of the particle from MMS and/or aircraft navigation data.

JouleMtr (relative units): A measure of the excimer laser power for the laser pulse for each particle. Note that even for identical joule meter values individual particles might be in more or less intense portions of the excimer laser beam.

ExcimerND (fraction): The value of a neutral density filter in the excimer beam. 1.0 means no filter and is the usual operating condition. Values near 0.75 or 0.8 are from a filter that was sometimes used to reduce the laser power after a fresh excimer gas fill to make it more comparable to other flights. Values near 0.2 are when the laser power was deliberately reduced to explore how ionization patterns changed with laser power. The effect of ExcimerND is reflected in the JouleMtr variable.

TrigScatHt (relative units): The size of the optical pulse when the particle scattered light as it went through the second 405 nm laser beam that is used to trigger the excimer laser.

TimingScatHt (relative units): The size of the optical pulse when the particle scattered light as it went through the first 405 nm laser beam. Not every particle has a timing signal. Timing scatter pulses can be compared to other timing scatter pulses but are on a different scale than the trigger scatter pulses.

AeroDiam (μm): The aerodynamic diameter of the particle derived from the time between the timing and trigger scatter signals. The PALMS inlet pressure is such that particles smaller than a few microns in diameter are in the free molecular flow regime where the aerodynamic diameter is proportional to density. The very largest particles are in a transition regime where density enters to a power between 0.5 and 1. A shape factor also enters into the aerodynamic diameter.

FlagBioBurn, FlagKRich, FlagMinMet, FlagSoot, FlagSeaSalt, FlagSulfOrg (0 or 1). These are flags, primarily for the positive ion spectra, to show if a particle was identified by automated criteria as a biomass burning particle, an alkali-rich particle, a mineral or metal particle, a soot particle, a sea salt particle, or a sulfate-organic-nitrate mixture. These categories are neither complete (some particles are not in any of these classes) nor exclusive (for example some sulfate-organic particles are biomass burning particles).

MassScaleA, MassScaleB (μs , $\mu\text{s Da}^{-0.5}$): These are the constants in an equation to convert ion arrival time to mass: $\text{time} = A + B \cdot \sqrt{\text{mass}}$. PALMS data processing fits this equation to each mass spectrum.

MScaleFitVariance (Da^2): The variance when the positions of the peaks are fit to the mass scale equation using integer values for the peak positions. At PALMS mass resolution there is often about a 0.1 Da uncertainty in the peak center. Exact masses are also often about 0.1 Da from an integer. A variance of about 0.01 therefore represents a near-perfect mass scale. Significantly higher variances usually indicate wide peaks from ionization effects in the mass spectra of dust and other refractory particles.

NumPks: The number of peaks in the mass spectrum.

TotalMCPSignal (electrons): The total signal from the microchannel plate (MCP) integrated over all peaks in the mass spectrum. The PALMS MCP is run at a relatively low gain of a few thousand and the gain is slightly different for positive and negative ion spectra.

AreasNoID (fraction): The areas of all peaks for which no mass number was assigned. This is usually zero. An example of a rare instance of a peak with no assigned mass is if the software can't decide if a local maximum is a separate peak or a shoulder on a larger peak.

AreasNonInt (fraction): The areas of all peaks with half-mass or other non-integer peak identification. In the PALMS ionization we rarely or never see doubly charged peaks from molecular ions. Even from elemental ions doubly charged peaks are usually very small. The most common is probably 25.5 from V⁺⁺. Intense sea-salt spectra sometimes have Na⁺⁺.

TotalMCPBackground (electrons): There is a very small ion background in PALMS in the positive ion mode, mostly at $m/z=12$. This is the value that was subtracted to obtain TotalMCPSignal.

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Altitude, latitude, and longitude courtesy of the MMS and aircraft navigation data teams. Excluding thick clouds utilized data from the CAPS Vienna team.