TITLE: Fast dimethylsulfide (DMS)

AUTHORS:

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1.0 DATA SET OVERVIEW:

Fast (25 Hz) and decimated 10 second dimethylsulfide (DMS) data for the Pacific Atmospheric Sulfur Experiment (PASE). Collected on the NCAR C-130 in Aug-Sept, 2007 from Kiritimati (Christmas) Island, Republic of Kiribati.

2.0 INSTRUMENT DESCRIPTION:

DMS measurements were obtained in positive ion mode with an Atmospheric Pressure Ionization Mass Spectrometer (APIMS, Bandy 2002). An isotopically labeled standard (d3-DMS) is added continuously to the sample air at the inlet. Protonated molecular ions at mass 63 (DMS•H+) and mass 66 (d3-DMS•H+) are monitored sequentially. Signal intensities are recorded as total ion counts in a 20 ms interval at each mass. The ambient DMS concentration is calculated from the signal ratio (mass63/mass66), the flow rate and concentration of labeled standard, and the total sample air flow rate. DMS concentrations are reported as parts-per-trillion by volume (pptv) or pL/L.

Two cylinders of isotopically labeled DMS used for the field program were each calibrated against two DMS permeation tubes maintained in the lab at Drexel University. Final calibration data for the standards yield concentrations of 101 ppb +/- 6% and 103 ppb +/- 6%. Including flow rate uncertainty, precision of the mean DMS concentration in the atmospheric boundary layer is therefore about 10%.

Instrument backgrounds (blanks) are obtained by passing sample air over a column of gold coated glass beads, removing DMS from the ambient sample stream. Background count rates at masses 63 and 66 are typically low (< 5% of total signal in the atmospheric boundary layer) and are subtracted from total counts before calculating the DMS concentration. Blank measurements are deleted from the data record and recorded as NaN in the final data file. In addition to blanks, other periods of data were lost due to electronic problems with the mass spectrometer RF power supply. These periods also appear in the data record as NaN.

3.0 DATA COLLECTION AND PROCESSING:

DMS concentrations at 25 Hz were computed from the raw data, and periods of bad data removed as described above. In addition, noise spikes from the ion multiplier were removed using a 25 point (1 second) median filter: data points in a sliding 25 point window exceeding the median value by more than 40 pptv were replaced with the median value. This filter seemed to do an adequate job removing occasional noise spikes without affecting the noise band significantly.

Fast (25 Hz) data was further decimated to 10 second intervals as a convenience for users who do not require high rate data.

4.0 DATA FORMAT:

Fast data for each flight is supplied in a series of files which roughly correspond to each individual flight leg. In addition to DMS concentration data and the UCAR time stamp, each file also includes the time stamp in text format (MM/DD/YYYY hh:mm:ss.sss) and Matlab datenumber decimal format:

```
PI/DATA CONTACT = Bandy, Alan (Drexel Univ.), Blomquist, Byron (Univ. Hawaii)
DATA COVERAGE = START: 0813201825; STOP: 0813202333 UTC
PLATFORM/SITE = C-130
```

```
INSTRUMENT = Atmospheric Pressure Ionization Mass Spectrometer (APIMS)
LOCATION = mobile
DATA VERSION = 1.0 (11 DEC 2007)
REMARKS = Pacific Atmospheric Sulfur Experiment (PASE)
REMARKS = DMS in parts per trillion by volume, pptv = pL/L
REMARKS = Time in UTC, Missing data = NaN
UTC  Timestamps MatlabTime DMS
UTC  UTC  UTC  pptv
20070813201825.5050  8/13/07 20:18:25.505 733267.8461285301    73
20070813201825.5450  8/13/07 20:18:25.545 733267.8461289931    99
20070813201825.5850  8/13/07 20:18:25.585 733267.8461294557    83
...
```

File names are structured as (for example): `RF03_20070813T201825_DMS_v1.txt`, where flight number and start time are indicated as shown. Time format in the file name is yyyymmddThhmmss (ISO 8601 format).

10 second data for each flight is supplied in a single file of similar structure. These files contain time stamp data in UCAR format and text string format (readable by most spreadsheet programs, Igor Pro, etc.).

```
PI/DATA CONTACT = Bandy, Alan (Drexel Univ.), Blomquist, Byron (Univ. Hawaii)
DATA COVERAGE = START: 0813183524; STOP: 0814021236 UTC
PLATFORM/SITE = C-130
INSTRUMENT = Atmospheric Pressure Ionization Mass Spectrometer (APIMS)
LOCATION = mobile
DATA VERSION = 1.0 (11 DEC 2007)
REMARKS = Pacific Atmospheric Sulfur Experiment (PASE)
REMARKS = DMS in parts per trillion by volume, pptv = pL/L
REMARKS = Time in UTC, Missing data = NaN
UTC  Timestamp DMS
UTC  UTC  pptv
20070813183524.3990  8/13/07 18:35:24.399 86
20070813183534.3990  8/13/07 18:35:34.399 86
20070813183544.3980  8/13/07 18:35:44.398 86
...
```

In addition to ascii data files, pdf notebook files for each flight contain notes and plots of each data segment to facilitate a "quick look" at individual flight legs.

5.0 DATA REMARKS:

For PASE the APIMS was configured with a suction (non-pressurized) inlet, since fast flux data was required. As a result of low and uncontrolled inlet pressures, instrument sensitivity decreases with altitude (ie. with lower pressure). Within the atmospheric boundary layer this effect is insignificant, but at higher altitudes the sensitivity drops to less than 20% of boundary layer performance. Instrument backgrounds can also change with altitude and humidity and are difficult to correct during rapidly changing profile legs. Because of decreased sensitivity, backgrounds are more significant at high altitude than in the boundary layer. This results in an occasional bias in mean DMS concentration of several parts per trillion during profiles at altitudes above the ABL.

6.0 REFERENCES:

Bandy, A., D. Thornton, F. Tu, B. Blomquist, W. Nadler, G. Mitchell, and D. Lenschow, Determination of the vertical flux of dimethyl sulfide by eddy correlation and atmospheric pressure ionization mass spectrometry (APIMS), Journal of Geophysical Research, 107 (D24), 4743 doi 10.1029/2002JD002472, 2002.