PTR-MS Readme File

John Shilling, PNNL, 7/1/2014

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\*\*Data uploaded on 7/16/14 have been converted to engineering units and have gone through initial QA/QC, but are not final data. Users of this “preliminary” data should be aware that it may change.\*\*

Please contact the instrument PI for any questions regarding this data. Please adhere to the ARM data policy when using this data. Note that suspected "bad" data and data when the instrument is zeroed may be retained in the file and flagged instead of deleted.

PTR-MS data was collected on an Ionicon high-sensitivity quadrupole mass spectrometer during the GoAmazon field campaign in the Manaus, Brazil region. The instrument was flown on the G1 research aircraft from February 18th to March 25th, 2014. The instrument was run in the ion monitoring mode in which discreet m/z values are scanned sequentially as part of a measurement cycle. The measurement period varied between 3.4 and 5 seconds during the campaign. Note that the scanned m/z channels varied during the campaign in an attempt to optimize sampling. Additional diagnostic channels were also scanned but are not included in the processed data files.

Instrument background has been subtracted by diverting the sample flow periodically through a catalytic converter which removed most VOCs from the airstream. Signal intensity is then converted to ppbv in one of three ways. m/z 33, 42, 45, 59, 69, 71, 79, 87, 93, 107, and 137 are calibrated using a gas calibration cylinder containing known concentrations of methanol, acetonitrile, acetaldehyde, acetone, isoprene, methacrolein, benzene, 3-methyl-buten-1-ol (prenol), toluene, m-xylene, and alpha-pinene respectively. m/z 61 concentrations are calculated using the literature reaction rate constants for acetic acid. Concentrations of m/z 75 and 83 are converted to ppbv by assuming a reaction rate of 2 x 10^-9. Attempts to compensate for possible interference have not been made. For many species, the background subtraction ultimately limits the accuracy of the measurements when concentrations are below 1 ppbv. Please contact the PI for more information about using data when concentrations are below 1ppbv. For some species, the data are reliable for concentrations <100 pptv, but for other species data at lower concentrations is much less reliable.

Data for m/z 43 are qualitative only because many species may contribute to the signal at this m/z. There is a higher degree of uncertainty associated with signal at m/z 61 because of its "stickiness" in the inlet and difficulty with routinely obtaining an accurate zero. There is a very high uncertainty associated with m/z 87 due to its high degree of fragmentation in the PTR-MS. In most cases,I expect the m/z 87 concentrations are significantly over estimated.

Files are in tab delimited text format. A one row header gives the column names including date and time as a single value, the m/z channel name, and a flag wave. Values listed in the m/z column are units of ppbv. The flag wave indicates instrument status. A flag value of 0 indicated normal operation, 1 indicates a zero period, 2 indicates bad data, and 3 indicates data when the pressure in the drift tube dropped below 2.2 mbar. Data with a 3 flag should not be used for quantitative analysis, but are generally acceptable for quantitative analysis.

Date and time are local time (Manaus, Brazil). The clock has been synced to the G-1 computer, though a hereto unquantified delay time exists as a result of sample transit from the inlet to the instrument.

The time stamp represents the beginning of the measurement cycle. Since the PTR-MS steps through the masses sequentially, the exact time a measurement has been made is a function of its position in the scan list, the averaging time, and the delay to account for voltage stepping. Please contact the PI if more accurate time stamps are necessary. m/z 69 has been sampled multiple times in one measurement cycle to enable flux analysis.

Additional notes on particular flight days:

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