PTR-MS Readme File

John Shilling, PNNL, 3/24/2015

PI contact information:

John Shilling

Pacific Northwest National Laboratory, Atmospheric Sciences and Global Change Division

902 Battelle Blvd

MSIN K4-28

Richland, WA 99352

Ph: 509-375-6874

e-mail: John.shilling@pnnl.gov

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 September 6th to October 4th, 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 was approximately 3.4 seconds. 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 two ways. m/z 42, 45, 59, 69, 71, 79, 93 and 137 are calibrated using a gas calibration cylinder containing known concentrations of acetonitrile, acetaldehyde, acetone, isoprene, methacrolein, benzene, toluene, and alpha-pinene respectively. The signal at m/z 75 was calibrated by assuming a H3O+/VOC reaction rate constant of 2 x10^9. 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.

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 qualitative 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:

September 6th: PTR-MS data not available due to rupture of one part of the vacuum line.

September 21st: Drift tube pressure was problematic during a portion of the flight. Note flag wave.

September 22nd: Drift tube pressure was problematic during a portion of the flight. Note flag wave.

October 1st: A large portion of the data from the beginning of the flight is not usable due to problems with the water flow controller. Note flag wave.