PTR-MS / PTR-TOF-MS
VOC fluxes during NOMAADS

NCAR, NOAA, NILU, UIBK
Proton transfer reaction

\[ H_3O^+ + VOC \xrightarrow{k} VOCH^+ + H_2O \]

Calculation of the neutral concentration

\[ [VOC] \approx \frac{1}{k \cdot t} \cdot \frac{cps(VOCH^+)}{cps(H_3O^+)} \]

Target compounds: Isoprene, isoprene oxidation products
PTR-MS

- Slides into 1 bay of C-130 rack
- 2\textsuperscript{nd} bay needed for additional options: i.e. inlet pump, calgas
- HIMIL inlet on C-130 requested
- For EC flux measurements we can only monitor 2-3 compounds (i.e. isoprene, MVK+MAC and perhaps Meoh or MT)
Rack during Mirage

MIRAGE/INTEX-B

Note: For NOMAADS we will need to request space adjacent to PTRMS for inlet pump and calibration unit
Alternative or complimentary

• Due to a broader chemistry focus of NOMAADS, a PTR-TOF-MS is proposed to be flown in collaboration between NILU, NOAA, UIBK and NCAR instead or along with PTR-MS

• Instrument comes already prepackaged in a NASA P-3 rack

• Inlet requirements will be the same as for PTR-MS
PTR-TOF-MS

footprint

POWER: 120V/1000W
Weight: 600 lbs
PTR-MS (NCAR) vs PTR-TOF-MS (NILU/NOAA/UIBK/NCAR)

- PTR-TOF-MS advantages: no pre-selection of compounds needed – we can measure the entire mass spectrum at 10 Hz

- LOD: similar btw. PTR-TOF-MS and PTR-MS for a nominal mass (i.e. compound), but much lower for PTR-TOF-MS, when considering that the instrument scans over the entire mass range

- PTR-TOF-MS disadvantage: somewhat lower sensitivity, but probably acceptable for isoprene flux measurements

- PTR-TOF-MS will also have the option of a SRI (selective reagion ionization) capability
EC flux leg flight patterns

Will need 20 Hz data stream post-flight

- Horizontal gradients (land cover characterization)
- Vertical gradients (flux divergence measurements)
Altitude above ground – PBL height
Forest: fetch about 10 x PBL height

Sounding (up to 4000-7000 ft depending on PBL) at beginning and end of each profile
Sounding can be a “sawtooth” on the outbound leg, should be a spiral between consecutive profiles and a “saw tooth” on the inbound leg: climb rate 500 ft/min

1 track is about 30 minutes
Entire profile is about 1.5 hours at 70 m/s
Profiles flown during CABERNET
Flux divergence

Determine OH:
$4 \times 10^6$ molecules / cm$^3$

Surface flux

Entrainment flux

normalized flux

normalized flux

z/zi

isoprene

wT

qw
MEGAN - Model of Emissions of Gases and Aerosols from Nature
Flux processing (FFT and wavelet decomposition)
Flux divergence

Entrainment Flux

Flux profile = function of Dahmkoehler number $Da$

$Da = \frac{\text{mixing timescale}}{\text{chemical timescale}}$

Reactive compound

More reactive compound

Surface Flux

PBL top

$z/h$