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An Axial Time-of-flight Mass Spectrometer for Upper Atmospheric Measurements

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Research objectives

- Design a time-of-flight mass spectrometer (TOFMS) for accurate measurements of charged and neutral particles in the Mesoshpere/Lower thermosphere (MLT)
- Test microchannel plate (MCP) detectors in the laboratory to determine high pressure operating characteristics
- Achieve unit mass resolution of atmospheric species of interest with TOFMS
- Model instrument sensitivity and performance for a typical sounding rocket flight to the MLT

Introduction

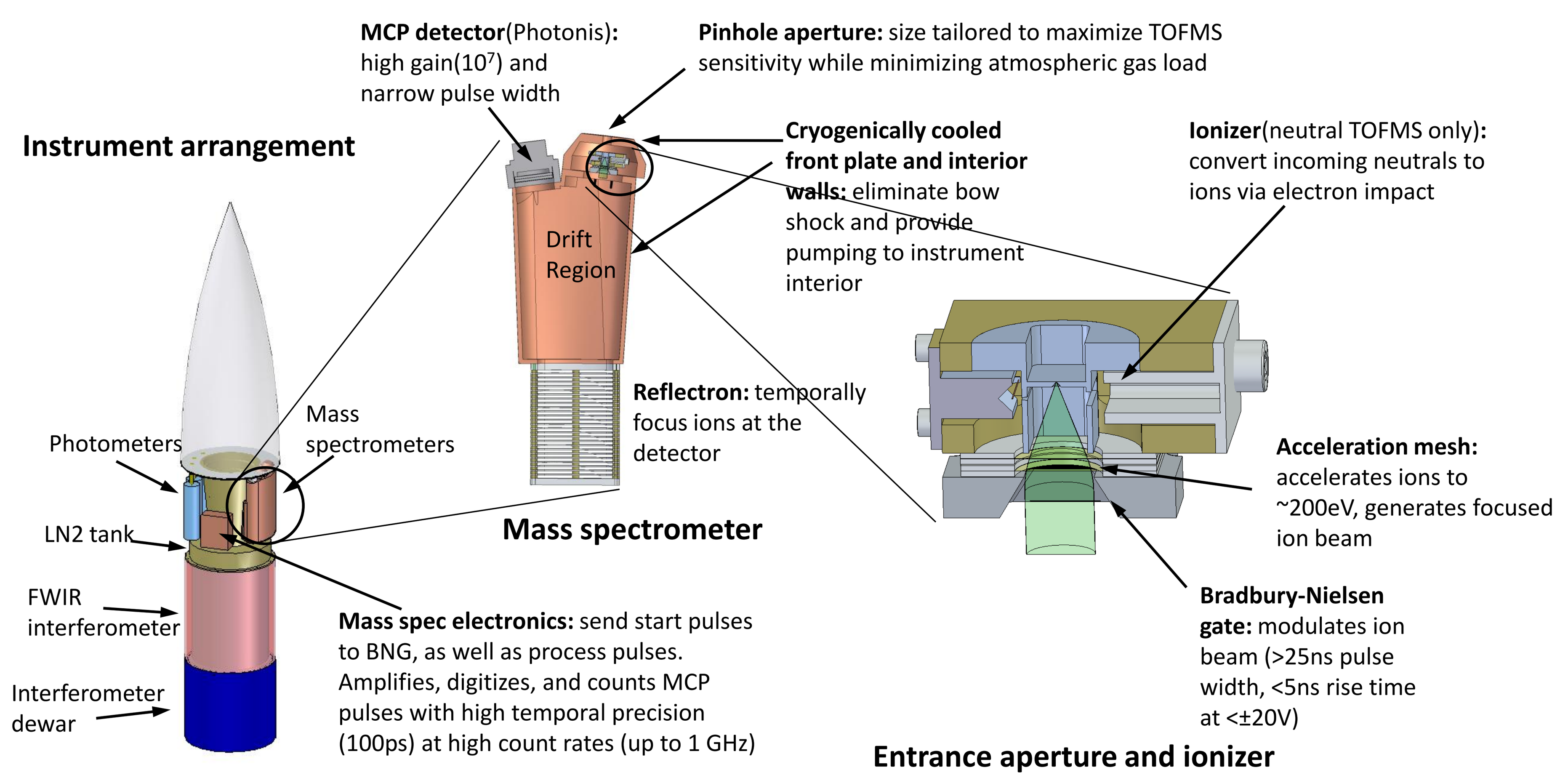
As the "shoreline" of the Earth's atmosphere, the mesosphere/lower thermosphere (MLT) region is home to many interesting and important phenomena, the most visible of which are the auroras. Geomagnetic storms, in addition to causing very intense auroral activity, also deposit large amounts of energy into the earth's ionosphere. Recent analysis of data from the Sounding of the Atmosphere using Broadband Emission Radiometry (SABER) instrument aboard the Thermosphere-Ionosphere-Mesosphere Energetics and Dynamics (TIMED) satellite suggests that 5.3μm emission from vibrationally excited NO is the main method of energy dissipation from energy deposited by geomagnetic storms. Additionally, NO^+ has been shown to be the major contributor to geomagnetic storm induced 4.3μm nighttime emission.

In order to better physically understand these two large sources of geomagnetic storm energy dissipation, a sounding rocket mission, **ROCK**et-borne **St**orm **E**nergetics of **A**uroral **D**osing in the **E**-region (**ROCK-STEADE**) is being proposed. The **ROCK-STEADE** instrument suite consists of several photometers, an interferometer, an IR spectrometer, and two time-of-flight mass spectrometers (TOFMS). The TOFMS will measure the ion and neutral compositions in the atmosphere as the sounding rocket travels through the MLT.

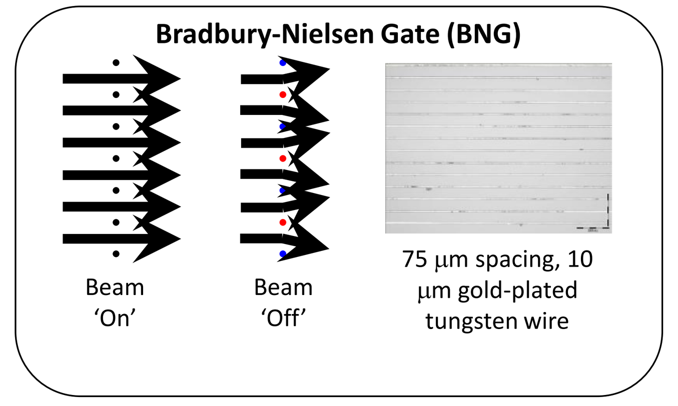
Due to the use of microchannel plate (MCP) detectors in TOFMS, one of the major challenges to making measurements in the MLT is the high ambient pressure. Other challenges and sources of error and background include stray UV photons, scattering of gas molecules from the interior surfaces of the instrument, dissociation of molecules in the bow shock caused by the supersonic rocket flight, and reactive recombination at the surfaces of the instrument. Methods of dealing with these challenges include:

- Recent advances in MCP technology allowing MCP operation into the mtorr range
- Cooling the front surface of the TOFMS using liquid He to eliminate the bow shock (thus making possible the direct sampling of the ambient atmosphere)
- Cryogenically cooling the interior of the instrument to eliminate scattering of gas from instrument walls and therefore also reducing the contribution of reactive recombination
- Rigorous error analysis to account for the background contribution of stray UV

ROCK-STEADE mass spectrometer



Mass spectrometry in the upper atmosphere

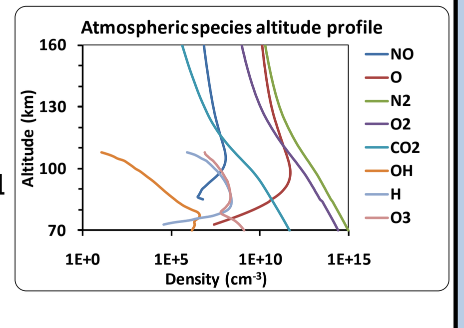


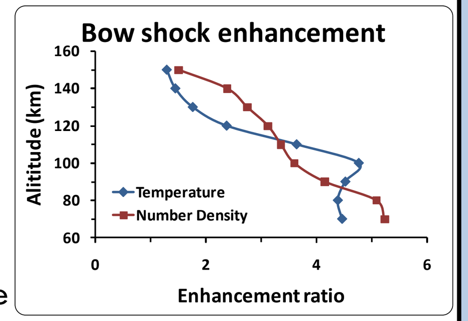
Well defined ion pulses are required for successful TOFMS in the MLT. This can be accomplished with a Bradbury-Nielsen gate (BNG) directly behind the ion acceleration region. A BNG consists of two inter-leaved sets of wires which, when set to the same potential as the acceleration mesh, allow uninhibited passage of charged particles. The ion beam is modulated by applying ±V to each set of wires, which serves to deflect the ion beam. The microscope image to the left shows a BNG fabricated "in house."

- Two interleaved sets of 10 μm diameter gold-plated tungsten wire, electrically isolated from each other
- 75 μm spacing between wires
- Very well defined, short pulses (>25ns pulse width, <5ns rise time)

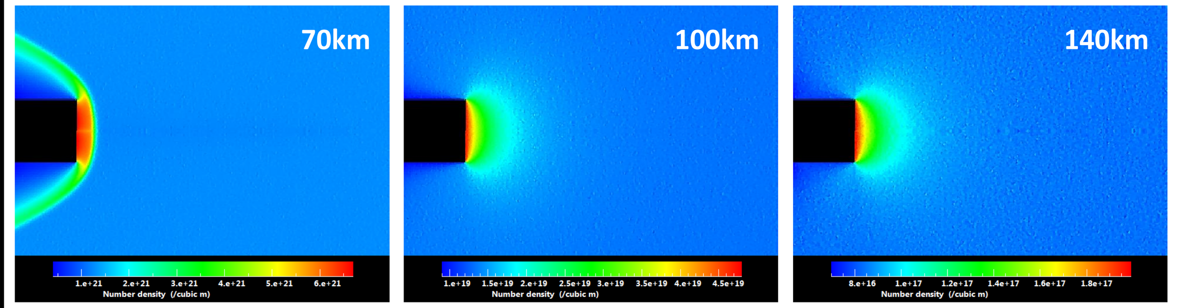
Challenges to taking mass spectrometer measurements in the MLT include:

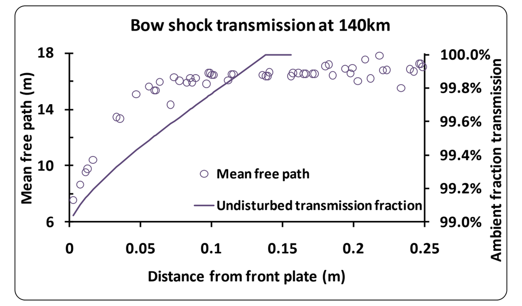
- **Pressure:** Pressures in the mesosphere/lower thermosphere can reach into the 10's of mtorr. This is a challenge for two reasons (1) a sufficiently long mean free path must be maintained inside the instrument and (2) pressure must be low enough to ensure successful MCP operation.
- **Bow shock:** High speed rocket flight causes a bow shock to form (see figures, below and right). Bow shock causes enhanced densities and pressures at the instrument entrance aperture. Bow shock heating can also cause dissociation of ambient molecules, thus making difficult the accurate measurement of ambient species.
- **Resolution of thin layers:** Certain atmospheric species form thin layers with thicknesses of up to several km. High instrument duty cycle and mass range are necessary to resolve these layers.
- **Wide variety of particles:** Particles of interest include both neutrals and ions. Particles range in mass from individual atoms (several amu) to smoke and dust particles (thousands of amu)
- **Background:** Sources of background include UV photons, detector dark counts and scattering of molecules from the interior walls of the detector.
- **Reactive species:** The largest contributor is O, which can react with contaminants on the walls of the instrument and subsequently be detected, leading to inaccurate interpretation of ambient species and number densities.

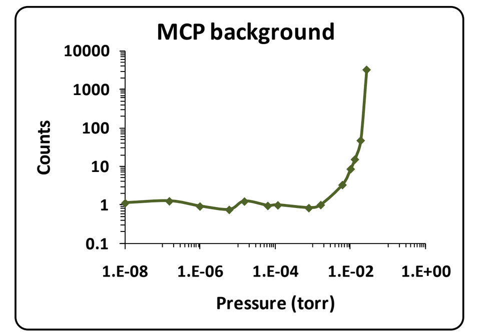


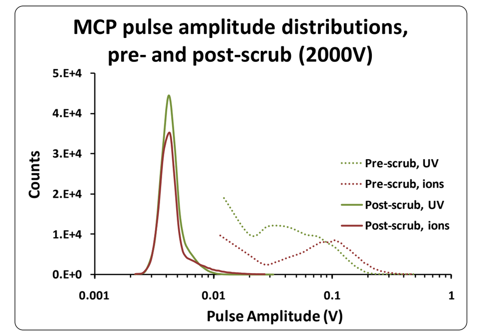


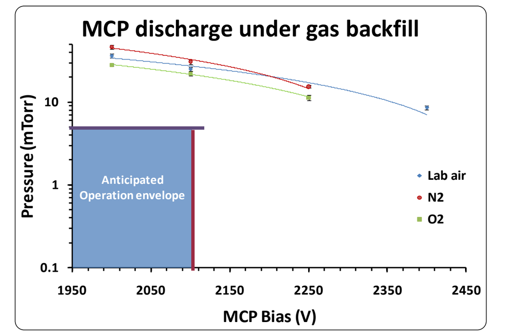
Images from Direct Simulation Monte Carlo modeling (below) show the number density enhancement that forms on the ram side of an instrument on a sounding rocket. **ROCK-STEADE** will use liquid He to cool the front plates of the mass spectrometers, as well as the interior walls of the instruments. This application of cryogen will effectively eliminate the bow shock while also pumping the instrument and adsorbing any stray gas molecules that impact the interior walls.





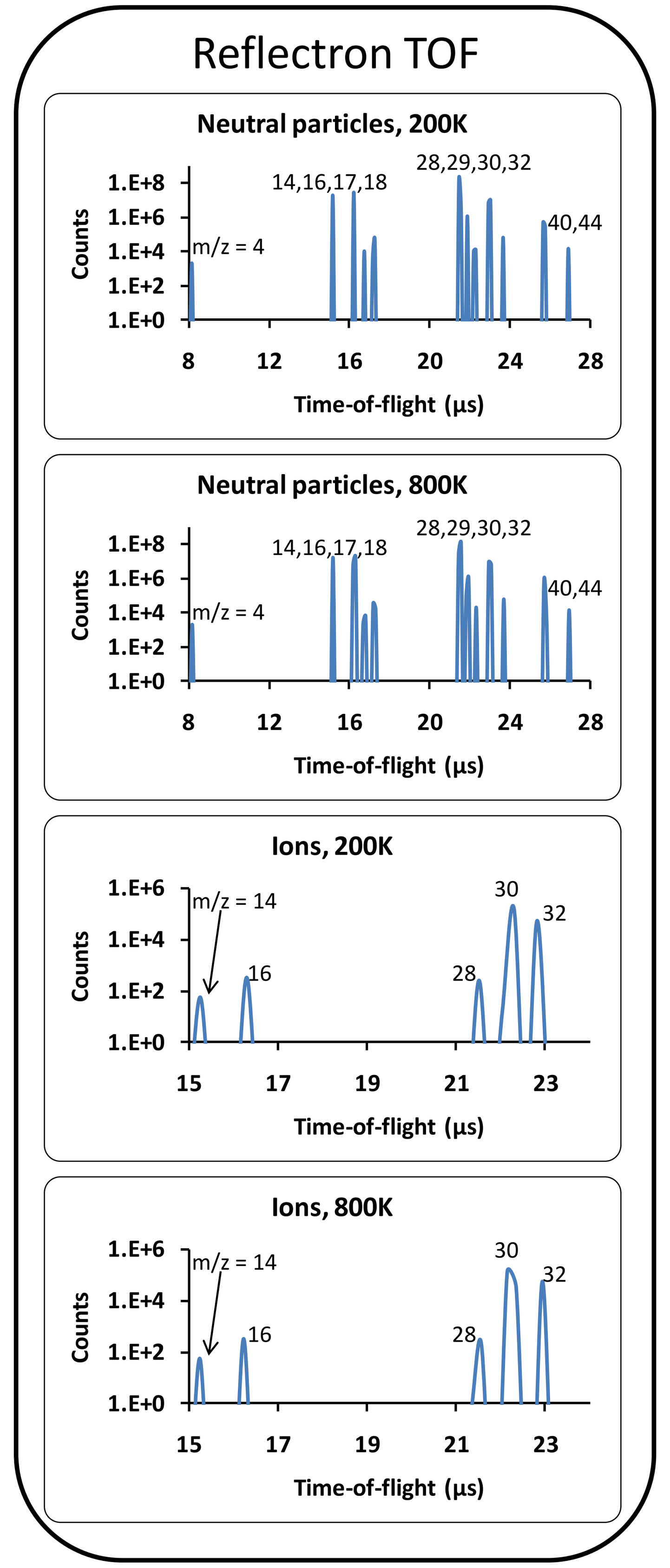


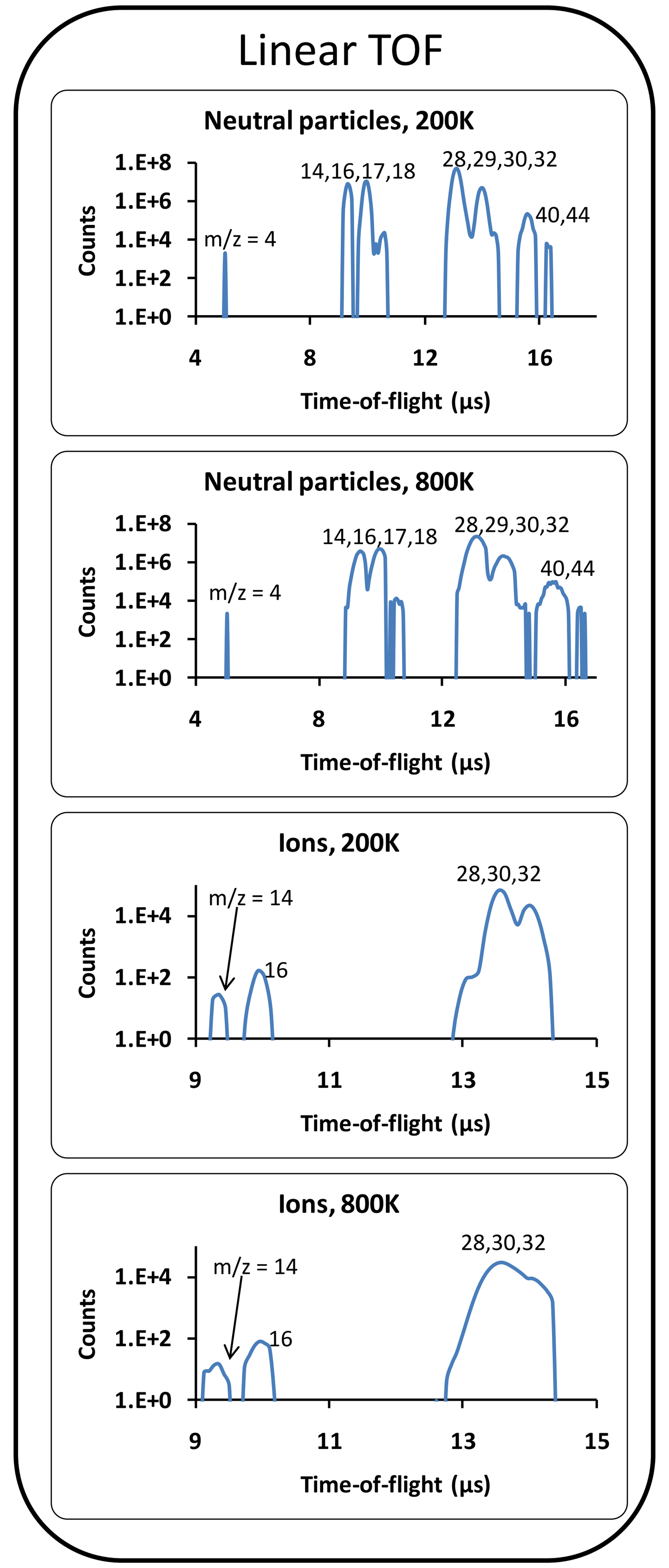




- High pressure MCP performance characteristics were demonstrated for N_2, O_2, Ar, He, and ambient lab air.
- Background count rates as a function of pressure show favorable MCP performance, even into the 10 mtorr range
- The pressures at which the MCP discharged for various gases was recorded. Note that all discharges occurred at pressures above the expected operating pressures of the instrument.
- Pre- and post-scrub pulse amplitudes were recorded for our MCP, at a potential of -2000V.

Predicted performance





Simulated instrument performance for number densities found at ~120km altitude. At 120km, ambient temperature is ~500K, however the above simulations were conducted assuming temperatures of 200K and 800K to show the peak spreading that results from higher KE of particles at high temperatures.

- Reflectron TOFMS drift lengths were
  - -20cm before and after the reflectron
  - -10cm penetration depth in the reflectron
- Linear TOFMS drift length was 50cm.
- Rocket velocity = 900m/s
- Aperture diameter = 1.5mm for neutral measurements and 25μm for ion measurements

Uncertainty analysis

The uncertainty in the number density of NO is given as an example of uncertainty analysis:

Begin with the variance for NO, which depends on:
- the uncertainty in the m = 30 peak,
- the uncertainty due to $N_2(30)$
- the uncertainty due to counts from stray UV

$$\sigma_{NO}^2 = \sigma_{30}^2 + \sigma_{N2(30)}^2 + \sigma_{UV}^2$$

For a function, $f = aA$, the variance of f is given by

$$\sigma_f^2 = a^2\sigma_A^2 .$$

For $\sigma_{N2(30)}^2$, the variance is

$$\sigma_{N2(30)}^2 = \left(0.0037^2\right)^2 \sigma_{N2(28)}^2 = \left(1.874\times10^{-10}\right)\sigma_{N2(28)}^2$$

where the factor of 0.0037 is the isotopic abundance of ^{15}N.
The uncertainty in a number of counts, N_A, is given by

$$\sigma_A = \sqrt{N_A}$$

which leads to

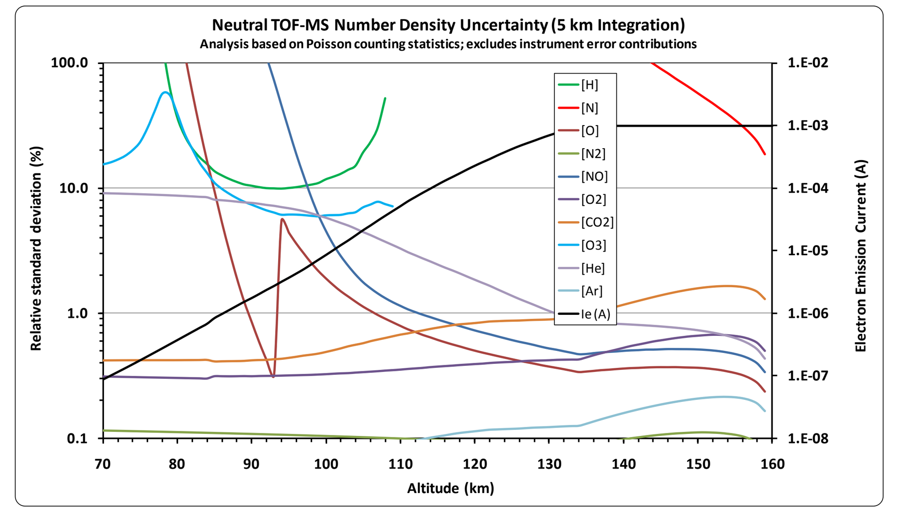
$$\sigma_{NO} = \sqrt{N_{30} + \left(1.874\times10^{-10}\right)N_{N2(28)} + N_{UV}}$$

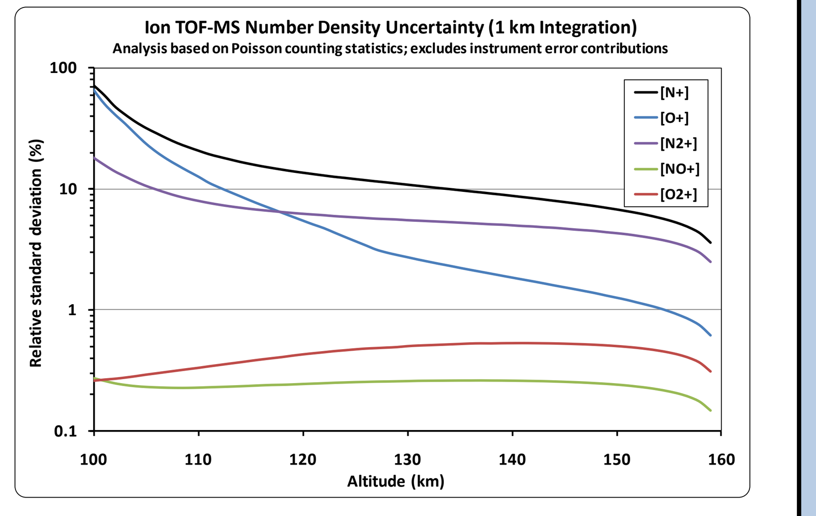
Dividing by N_{NO} gives the relative standard deviation (%)

$$\sigma_{NO} = 100\cdot\frac{\sqrt{N_{30} + \left(1.874\times10^{-10}\right)N_{N2(28)} + N_{UV}}}{N_{NO}}$$

Several factors affect the uncertainty and hence, sensitivity, of the instrument. Among them are:
- **Detector background**
- **Stray UV photons**
- **Dissociation of molecules**

m/z	Peak contributors
4	He
14	N (from atomic N, dissociated N_2 and, NO)
16	O(from atomic O, dissociated O_2, NO and CO_2)
17	OH and ^{17}O
18	^{18}O(from atomic ^{18}O, dissociated O_2, NO, and CO_2)
28	N_2 and CO from dissociated CO_2
29	N_2 (with one ^{15}N) and CO(with one ^{13}C from dissociated CO_2)
30	NO and N_2 (with two ^{15}N atoms)
32	O_2, NO (with one ^{18}O)
34	O_2, (two ^{17}O atoms)
40	Ar
44	CO_2





Conclusions

The simulations and experiments presented in this poster show the possibility of operating a simple TOF mass spectrometer as part of an instrument suite on a sounding rocket mission to the mesosphere/lower thermosphere. A compact time-of-flight instrument such as the instrument presented can be employed to make fast, accurate measurements of atmospheric species of interest. Specifically, these results show that:

- An MCP detector can be successfully operated at the pressures encountered on a sounding rocket flight to the MLT
- Mass resolution in our instrument is greatly improved by employing a reflectron
- Instrument sensitivity will allow accurate measurement of atmospheric species

Acknowledgments

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