Mass Spectrometry of the Turbopause Region (MSTR)
A High-Performance Cryogenic Time of Flight Mass Spectrometer for the Space Community

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SUMMARY

The chemistry and dynamics of the Turbopause, 80-120 km, profoundly affect the global and regional climatological behavior of the thermosphere-ionosphere system. A detailed understanding of this region is critical to modeling and predicting extreme, high-altitude weather systems, which can have a detrimental effect on space and ground-based products. Our knowledge of this region remains poor and is further complicated by the fact that accessing the Turbopause, in situ, is difficult and must rely on rocket flights. To improve our understanding of this critical region, we present the Mass Spectrometry of the Turbopause Region (MSTR) instrument, a novel, cryogenically cooled Time-Of-Flight mass spectrometer (CTOF-MS) for the first modern, simultaneous composition measurements of O, O_2, N_2, N_O, CO_2, H_2O, O_3, and Ar, for the Turbopause region. MSTR is a compact, high-resolution (>3000) TOF-MS payload, designed for Small Satellite and sounding rocket platforms. MSTR is currently planned to integrate with a low-altitude sounding rocket and features a helium-cooled cryogenic nose cone that will reduce and collapse the impinging bow shock of the supersonic rocket. The goal of the MSTR program is to directly study, in situ, the chemistry and dynamics of the Turbopause region. The MSTR instrument is planned to launch from Poker Flatts during polar winter and will operate coincidentally with ground-based LIDAR and remote sensing overflights from SABER to resolve the complex temporal-spatial dynamics of the Turbopause region. Future flights of the MSTR payload will provide valuable benchmark data to validate Global Circulation Models (GCM) such as WACCM, Thermosphere-Ionosphere-Mesosphere-Electrodynamics GCM (TIME-GCM), and Whole Atmosphere Model (WAM). The MSTR instrument is a NASA HTIDS-funded technology development effort led by Orion Space Solutions (OSS) and Southwest Research Institute (SwRI).

Science Questions:

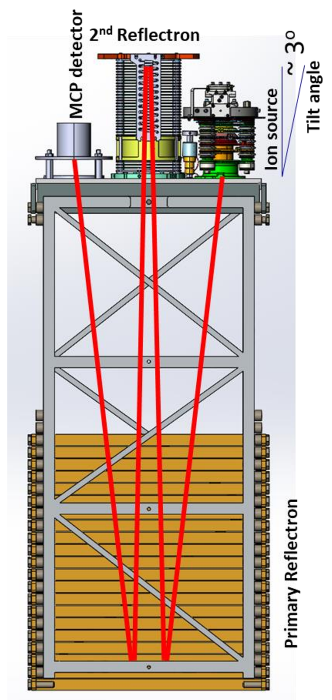
Question. #1: **What is the composition and structure of the Turbopause region as a function of altitude Relative profiles of O, O2, N2, NO, CO2, H2O, and Ar volume densities as a function of altitude**

Question #2: **Compare in-situ measured CO2 profiles (80-120 km) with those retrieved by IR radiometry at high latitudes during polar night**

Question. #3: **Measure the NO transport across the Turbopause, during the polar night.**

TIME OF FLIGHT MASS SPECTROMETRY

- Ion packets accelerated with uniform kinetic energy and time required to move through a fixed distance is measured.
- $KE = \frac{1}{2}mv^2$, lighter ions travel faster than heavier ones and get mass separation
- The greater the distance between the source and detector, the greater the mass resolution (ability to separate small mass differences between ions)
- To achieve greater distances between the source and detector without increasing length (footprint), the ion optics must be folded.
- Over the course of the MSTR program, we have developed a V-TOF-MS (single reflectron) and W-TOF-MS (multiple reflectron for W-shaped flight path).
  - W-TOF-MS CAD drawing shown at right with ion flight path (trajectory) in red.
- V-TOF and W-TOF-MS both have neutral and ion analysis capability.
  - Employ a Bradbury-Nielsen gate (BNG) for ion mode analysis
- Mass resolution driving requirements for future sounding rocket flights:
  - Resolution of CO^+ versus N_2^+ at nominal $m/z = 28$ (Mass resolution > 2,500)
  - Resolution of Ar^{++} versus Ne^+ at nominal $m/z = 20$

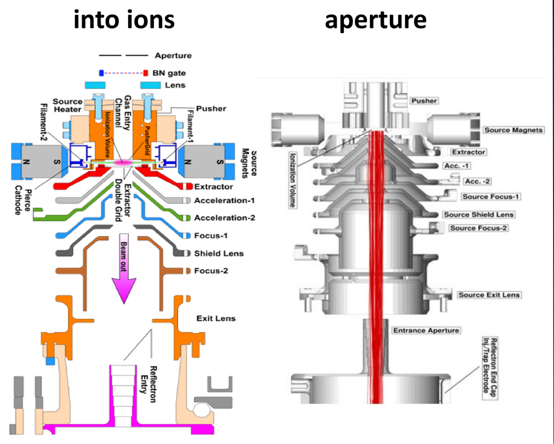


W-TOF-MS currently under development.

INSTRUMENT DESIGN

Two-stage gridless rectangular reflectron consisting of 21 field forming rings and a field-free drift region. An electron ionization storage source is employed for ionization of incoming neutrals, and a coaxially arranged Bradbury-Neilsen ion gate is employed for the analysis of incoming ions. A microchannel plate is used for registering the mass ions after extraction from the source(s)
The CTOF is fitted with a spare flight-qualified (MASPEX-Europa) electron ionization, multi-stage storage ion source having two redundant filament assemblies, low aberration acceleration and focusing elements, open, axial neutral/ion gas entry channel for ions and neutrals to enter from the cryogenic bow shock reducer.
The electron ionization source employs ion storage capabilities thereby increasing the source sensitivity
When tested, the V-TOF design exceeded resolution requirements and we have added an additional small static reflectron to fold the flight path into a W-path, further increasing the resolving power while maintaining the same instrument footprint
The additional resolution of the W-TOT will allow the separation of near-mass compounds such as CO, N_2, C_2H_4, (27.9949, 28.0061, 28.0313 u), and make accurate mass measurements to differentiate nearly isobaric mass ions with higher precision

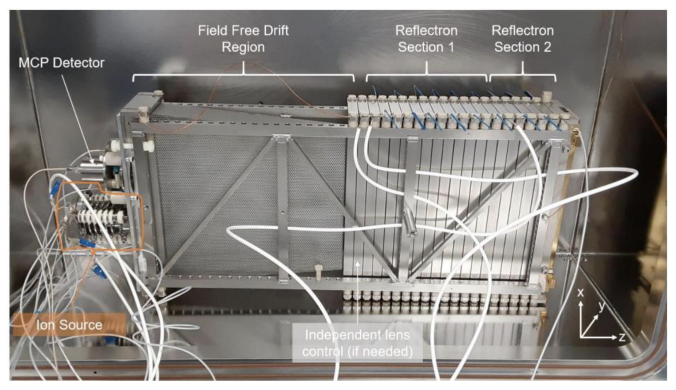
Neutrals formed into ions **5 mm diameter aperture**



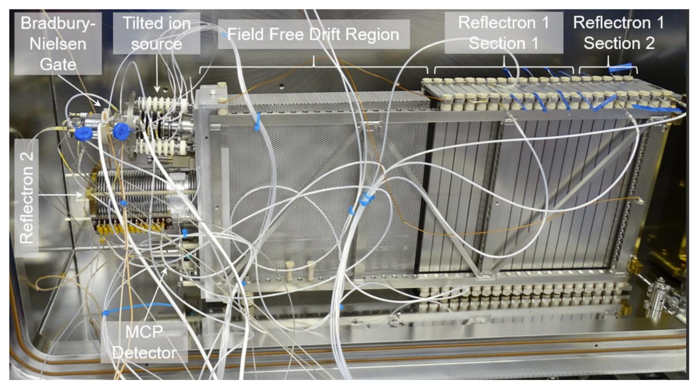
MSTR Electron ionization storage time-of-flight source with simulated ion trajectories. Left panel shows relative position of the aperture and BN gate. The gas entry channel allows direct entry to the ionization region.

PERFORMANCE

- V-TOF and W-TOF-MS have been tested to determine performance for the following analytical figures of merit:
- Two photographs of the two TOF mass spectrometer designs are displayed below
  - Mass resolution, Sensitivity, Dynamic Range, Isotope Ratio Measurement Accuracy
- A variety of gases (samples) have been tested with both the V-TOF and W-TOF-MS instruments
- Featured below is a noble gas mixture including: helium (He), neon (Ne), argon (Ar), krypton (Kr), and xenon (Xe)



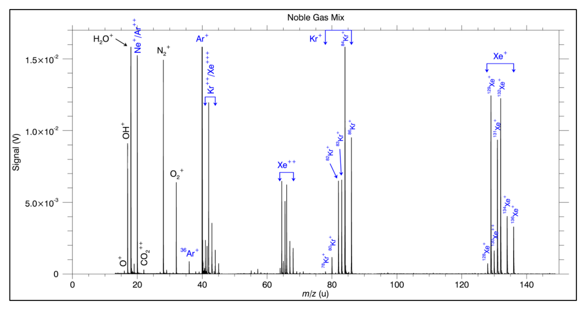
Photograph of V-TOF-MS with labeled components in the TOF development vacuum chamber.



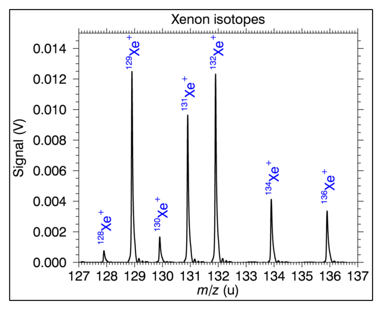
Photograph of W-TOF-MS and Bradbury-Nielsen gate (BNG) incorporated on the neutral ion source currently under development.

REFRENCES

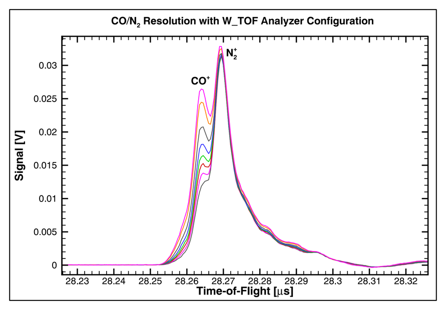
1. Aikin, A. C., A. E. Hedin, D. J. Kendig, and S. Drake, Thermospheric molecular oxygen measurements using the ultraviolet spectrometer on the Solar Maximum Mission spacecraft, J. Geophys. Res., 98(A10), 17,607, 1993
2. Allen, M., Y. L. Yung, and J. W. Waters, Vertical transport and photochemistry in the terrestrial mesosphere and lower thermosphere (50-120 km), J. Geophys. Res., 86, 3617-3627, 1981.
3. Andrews, D. G., J. R. Holton, and C. B. Leovy, Middle atmosphere dynamics, 489 pp., Academic Press Inc., New York, 1987.
4. Offermann, D., V. Friedrich, P. Ross, and U. Von Zahn, Neutral gas composition measurements between 80 and 120 km, Planet. Space Sci., 29, 747–764, 1981.
5. Offermann, D. and H. Tatarczyk, Cryo-cooled mass spectrometer ion source for atmospheric composition measurements at supersonic rocket velocities, Review of Scientific Instruments, 44, 1569-72, 1973.



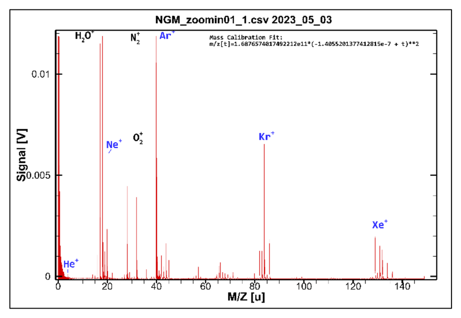
Mass spectrum of a noble gas mixture – He, Ne, Ar, Kr, Xe - recorded by W-TOF-MS. Noble gas ion signals labeled in blue, background residual gas labeled in black.



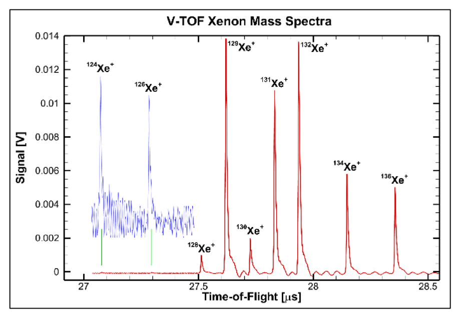
Zoom-in view of the Xenon isotopes recorded by W-TOF-MS.



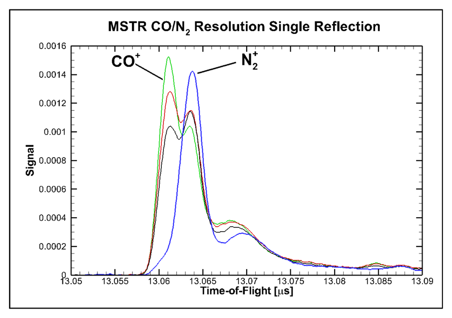
TOF spectra displaying doublet of CO^+ (27.99435 u) and N_2^+ (28.0055 u) as measured by the W-TOF MS.



Mass spectrum of noble gas mixture – He, Ne, Ar, Kr, Xe - recorded by V-TOF-MS.

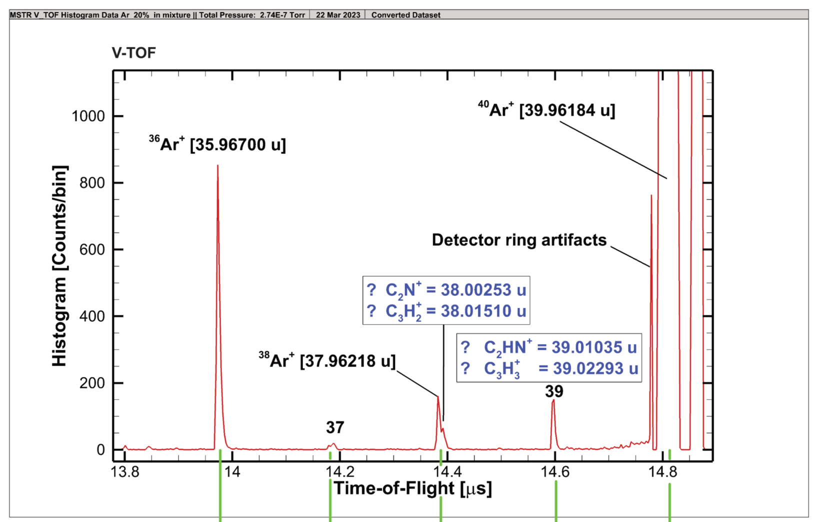


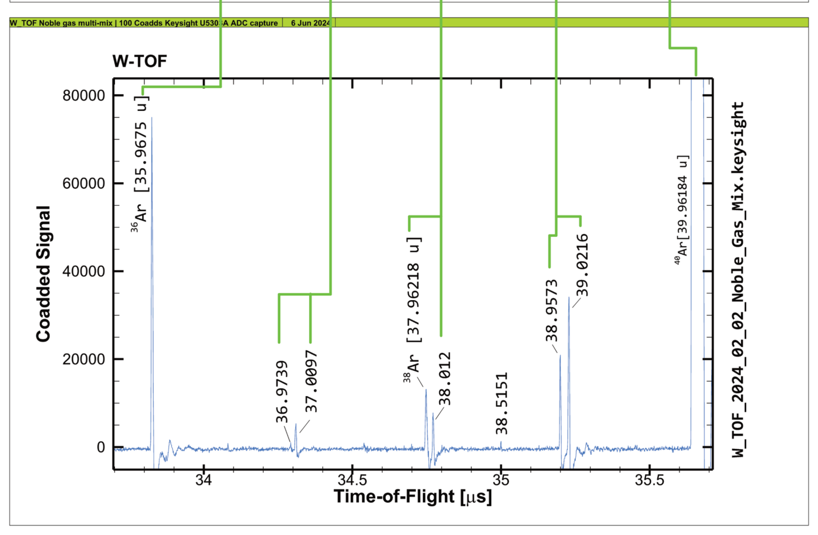
View of the Xenon isotopes recorded by V-TOF-MS. Blue inset shows further zoom-in of $^{124}Xe^+$ and $^{126}Xe^+$ isotopes showcasing dynamic range.



TOF spectra displaying doublet of CO^+ (27.99435 u) and N_2^+ (28.0055 u) measured by V-TOF MS.

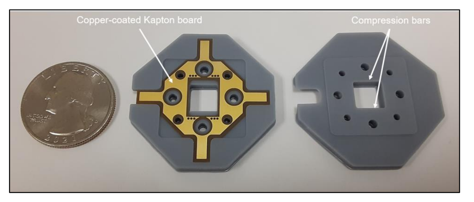
Right: The improved resolution helps quantify the isotopic ratio of the minor argon isotopes in this example there is some interference with the 38Ar isotope with some unknown in the spectra.



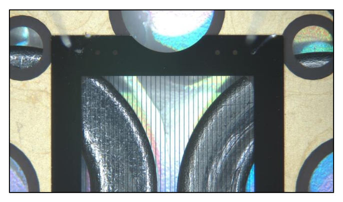


BRADBURY-NIELSEN GATE (BNG)

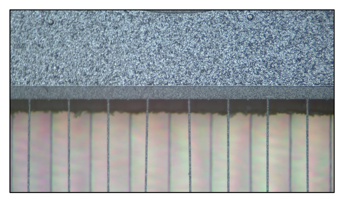
- For ion mode analysis, a Bradbury-Nielsen gate (BNG) serves as an ion gating mechanism for admitting narrow ion packets.
- Electroformed Ni harp wires are mounted on two sides of a copper (or gold)-coated Kapton board.
- Wires on opposite sides of Kapton board are interleaved so adjacent wires can be gate:
  - Held at opposite (differing) potentials to create an electric field to block the ion beam – Gate closed
  - Pulsed to the same potential to create a field free region that the ion beam can pass through – Gate open



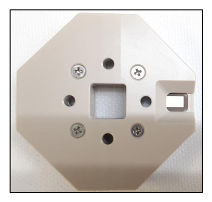
Photograph of Kapton board inside clam shell pieces to compress Ni harp wires of BNG into the same plane.



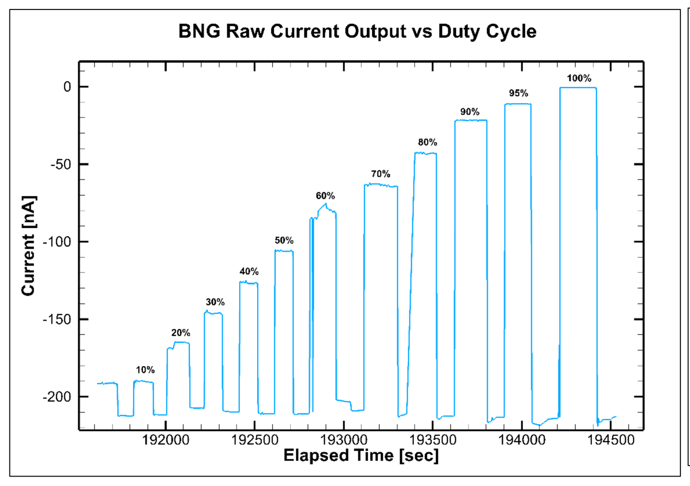
Photograph of one set of electroform Ni harp wires mounted on one side of Kapton board.

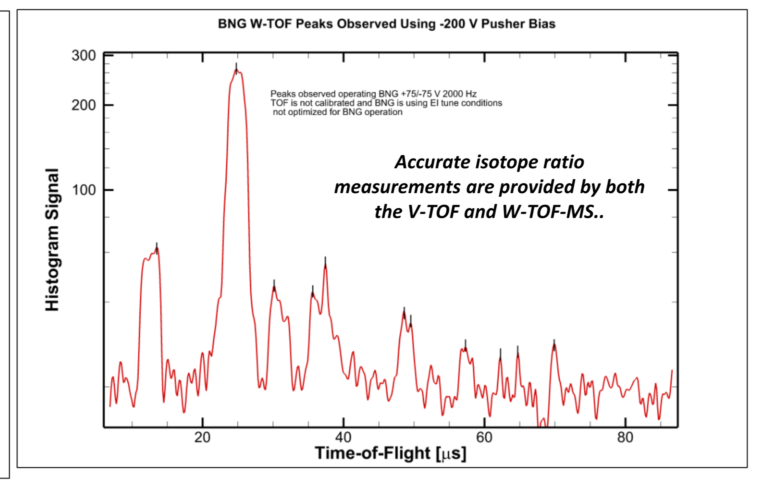


Photograph of both sets of Ni harp wires showing interleaved alignment prior to compression.



fully assembled and compressed BNG.





Left plot shows operation of BNG at various duty cycles. At 100% duty cycle (Gate Closed), no measured ion current. At 0% duty cycle, maximum ion current achieved. Duty cycle incremental steps investigated.

Plot at right showing first TOF spectrum obtained with BNG operation. Ions created with small ion source and gated into W-TOF-MS with BNG. Further optimization for improved performance is underway.

MSTR ADVANTAGES & DESIGN HIGHLIGHTS

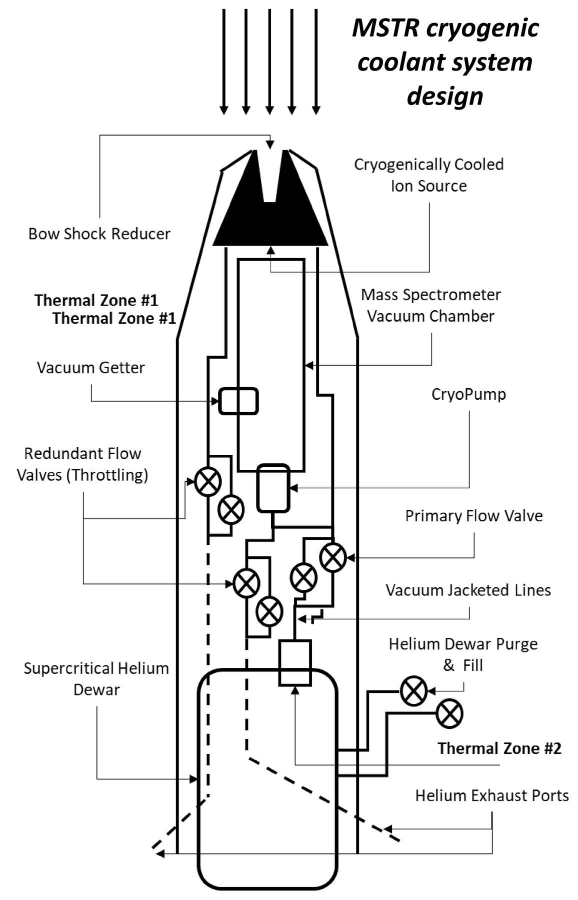
MSTR Design Summary	V-TOF	W-TOF
Mass (kg)	7.7 kg	8.1 kg (finalize #)
Dimensions (cm)	61 x 26 x 8.9	66 x 26 x 8.9
Cuboid Volume (cm^3)	14,115	15,272
Power (W)	<250*	15
Mass Resolution	1500-2500	2000-3500
Data Scan Rate	12-bit 1.6 GsPS ADC	12-bit 1.6 GsPS ADC
Atomic Mass	1-500u	1-500u

Xenon isotope	W-TOF	V-TOF	NIST reference ratio	Δ (% diff.) from NIST (W-TOF)	Δ (% diff.) from NIST (V-TOF)
$^{128}Xe^+$	0.0686	0.072	0.0705	-2.70 %	+2.13 %
$^{129}Xe^+$	0.980	1.059	0.984	-0.407 %	+7.62 %
$^{130}Xe^+$	0.145	0.151	0.152	-4.61 %	-0.658 %
$^{131}Xe^+$	0.784	0.801	0.794	-1.26 %	+0.882 %
$^{132}Xe^+$	1	1	1	N/A	N/A
$^{134}Xe^+$	0.380	0.388	0.378	+0.529 %	+2.65 %
$^{136}Xe^+$	0.322	0.334	0.320	+0.625 %	+4.38 %

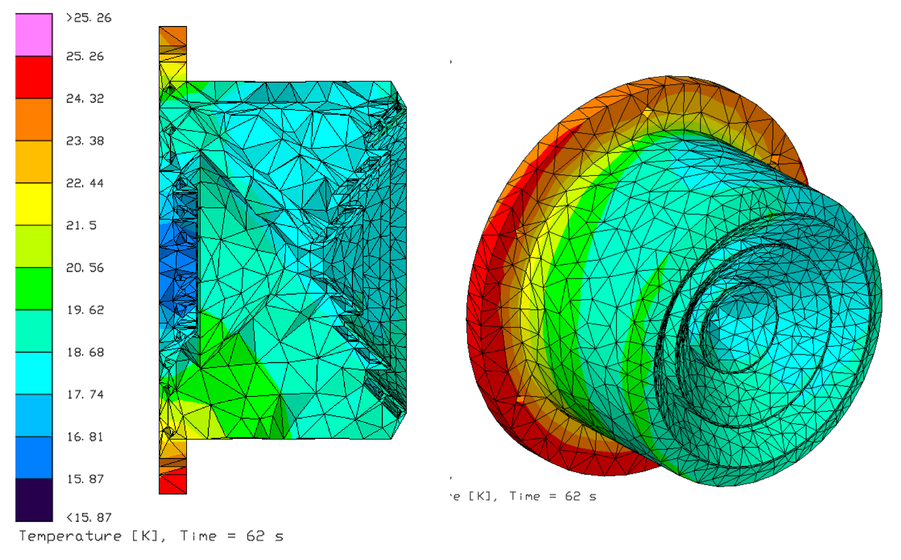
BOW SHOCK REDUCTION

During flight, the MSTR TOF-MS instrument will experience the formation of a bow shock and significant aerodynamic heating. To ensure that the payload can accurately sample the atmospheric environment a cryogenic nosecone will reduce and collapse the impinging bow-shock at the rocket nosecone. A 3D printed (DMLS GRCOP-42) cryogenic nosecone will be subcooled to <20 K during flight. The MSTR nosecone features embedded supercritical He coolant channels, a concave tiered design, and a secondary cooled chamber to prevent off-axis or reflected particles from entering the TOF-MS system. The thermal performance of the cryogenic system has been numerically modeled and verified in SimCryogenics, Thermal Desktop, and MolFlow.

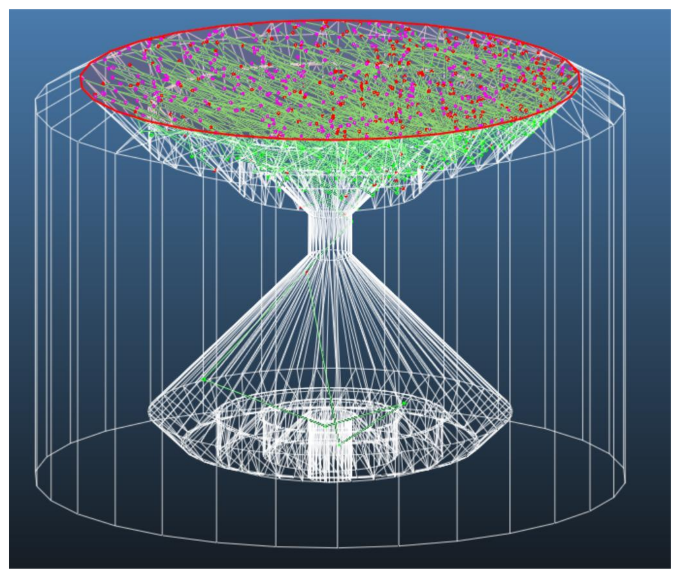
MSTR cryogenic coolant system design

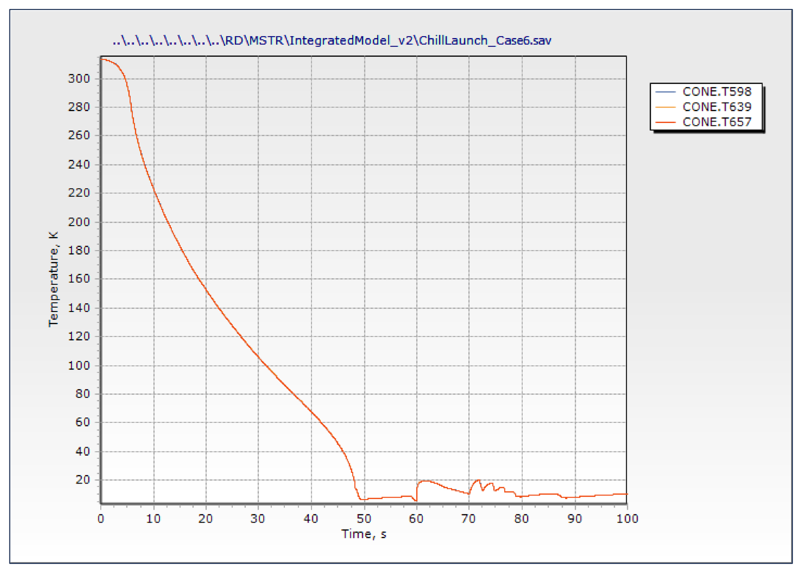


- Ram Heating >1.5 kW, initial loading
- Supercritical He Dewar
  - Pressurized to <6 atm
  - <20 K nosecone temperature
  - ~20-25 liters
- redundant flow control valves



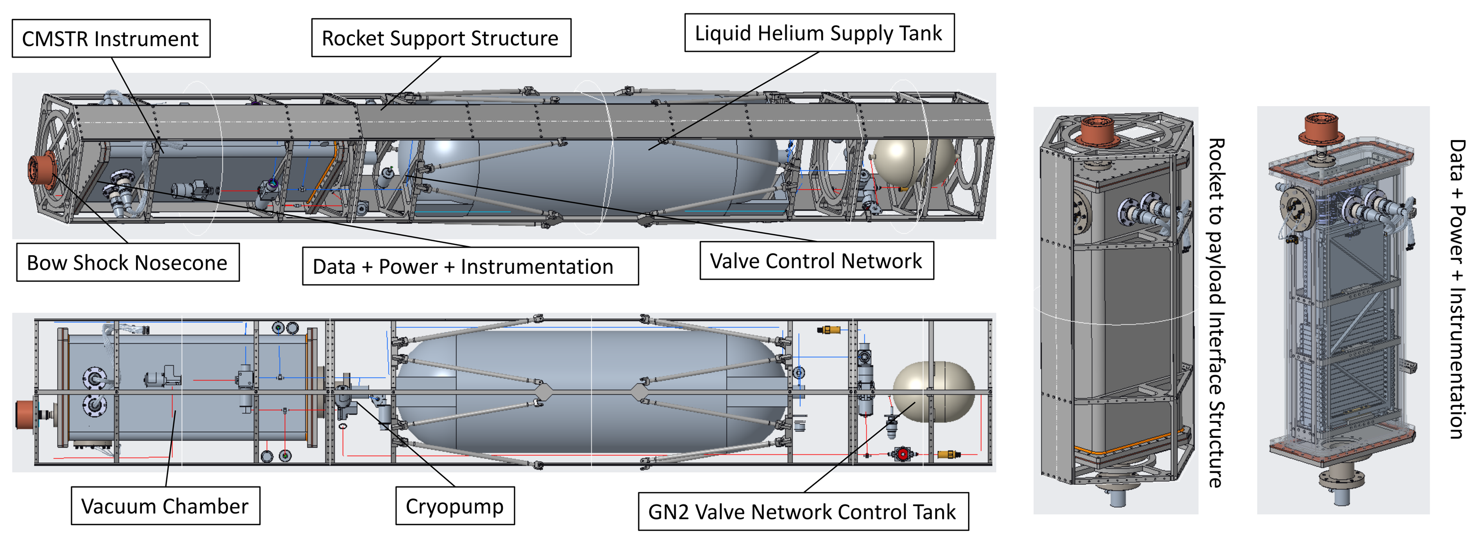
MolFlow simulation of the MSTR nosecone *Thermal performance of the MSTR nosecone*





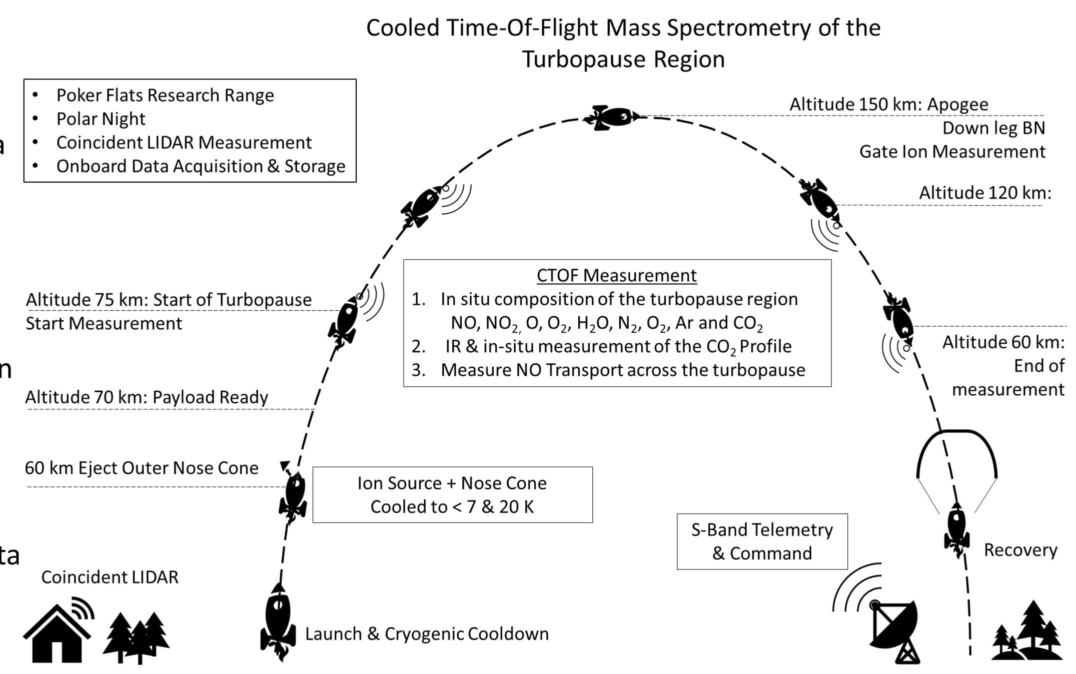
SOUNDING ROCKET MISSION CONCEPTS

The MSTR TOF-MS instrument will ideally launch from a high-latitude range, such as Poker Flats in Alaska, on or near the polar winter and *ideally* coincide with ground-based LIDAR measurements and SABER overflights. The MSTR flight concept includes in-situ data collection between 80 and 140 km, with neutral measurement on the up leg and ion sampling on the down leg. The MSTR instrument will be enclosed by a custom "Sleeve" vacuum chamber and attached to the cryogenic cooling system and an integrated cryo pump. The MSTR instrument is currently designed to fit in the elongated payload envelope defined by a standard-sounding rocket. A Black Brandt or Terrier (II) sounding rocket would be ideal.



- Poker Flats Research Range
- Polar Night
- High-Latitudes
- Chemistry data is collected via S-band downlink

<u>CONOP Steps:</u>
1. Launch
2. Instrument Ready
3. 1-70 km: Bow shock cooldown
4. 70 km: Eject outer nosecone
5. 75 km: Instrument ready
6. 75-150 km: Collect data
7. 150 km: Apogee
8. 150 km-60 km: Collect ion data
9. 60 km: Instrument shutdown
10. <50 km: Parachute deploy
11. Payload recovery



CONCLUSIONS

The MSTR-flight instrument is a compact ion and neutral time-of-flight mass spectrometer that includes a cryogenically cooled nosecone to sample the ambient atmosphere under high-velocity free flow conditions. This enables accurate and high-resolution, >3000, number density measurements of target neutral and ion species. The MSTR instrument is ideal for integration with a wide variety of flight vehicles, including sounding rockets, Small Satellites, and CubeSats.

The MSTR payload is currently under development by the teams at the Southwest Research Institute and Orion Space Solutions with funding through HTIDES and the NASA HESTO Office.

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