Apparatus Schematic Improvements and Vacuum Simulations for Astrochemical Experiments REU Program at Columbia University - Nevis Labs

Damien Algernon[1,2]

[1]Amherst College
[2]Nevis Labs

January 16, 2026

Nevis Laboratories
Columbia University

Abstract

This work supports the operation and development of the merged fast-beams apparatus at Columbia University, used to study ion-neutral reactions relevant to astrochemistry. I identified and helped resolve two gas leaks in supply lines, updated the three-dimensional Inventor model of the apparatus to match its as-built configuration, and began vacuum modeling work using Molflow+. These steps improve apparatus reliability, documentation, and vacuum understanding, which are all essential for precision measurements of reactions such as $N_2 + H_3^+$.

Contents

1 Introduction

Ion-neutral reactions involving molecular cations such as H_3^+ and its isotopologues are fundamental to the chemistry of cold interstellar environments and influence the evolution of molecular clouds into star- and planet-forming systems. In the very dense and cold conditions of prestellar cores and the outer regions of protoplanetary disks, deuterium fractionation is enhanced, producing abundance ratios of deuterated molecules far exceeding the cosmic D/H ratio [1]. This fractionation originates in barrierless, exoergic reactions by which HD deuterates H_3^+ to form H_2D^+, D_2H^+, and D_3^+, which then transfer deuteration to other molecular ions (e.g., N_2H^+ and N_2D^+) through subsequent ion-neutral reactions [2].

N_2H^+ and N_2D^+ are widely used tracers for cold dense gas and serve as chemical clocks to constrain the evolutionary stages of prestellar cores and the physical structure of protoplanetary disks [3, 4]. The reliability of these astronomical interpretations depends critically on accurate laboratory reaction kinetics for the isotopologues of H_3^+ reacting with N_2, as well as on understanding how internal excitation of the reactants influences reaction outcomes [5, 6].

The dual-source merged fast-beams apparatus at Columbia University is designed to measure ion-neutral reaction cross sections relevant to astrochemistry under well-controlled conditions. One ion source, a duoplasmatron, produces fast molecular ion beams such as H_3^+, generated through electron-impact ionization of H_2 followed by proton transfer. This process produces ions with significant internal excitation that can affect reaction outcomes [5]. Techniques including collisional relaxation and chemical destruction have been developed to control the internal energy of H_3^+ prior to interaction measurements, enabling studies of how vibrational and rotational excitation influence reaction rates [6]. The neutral beam is generated by collisions of a fast N_2^+ beam with cold N_2 gas inside the gas cell, and the two beams are merged with sub-milliradian precision in the interaction region, where product ions are analyzed using an electrostatic energy analyzer and a channel electron multiplier detector [7].

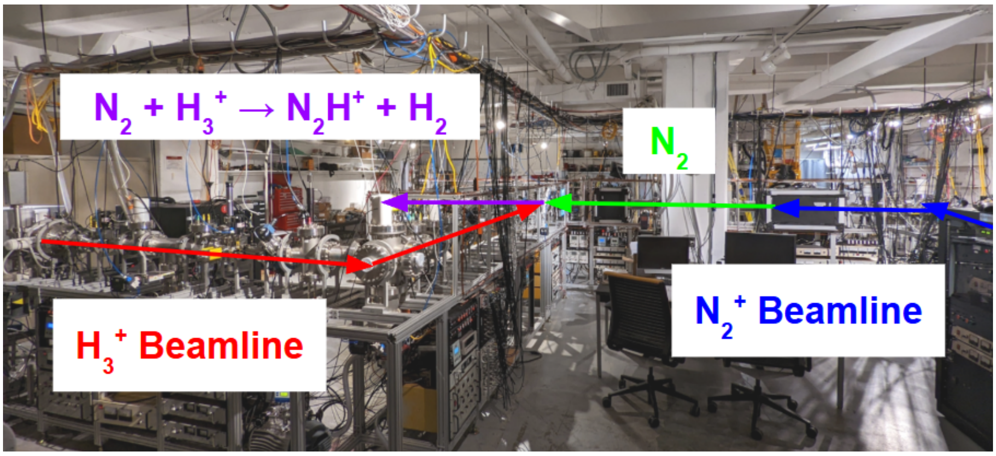

Figure 1: *Schematic of the dual-source merged fast-beams apparatus used to study ion-neutral reactions.*

The interaction of N_2 with H_3^+ is an important process driving the nitrogen chemistry of cold astrophysical environments. In prestellar and protostellar cores, where temperatures can drop below 20 K, reactions of H_3^+ with neutral species initiate networks leading to the formation of protonated and deuterated ions such as N_2H^+ and N_2D^+. These ions are widely used as tracers of cold dense gas because they resist freeze-out onto dust grains and preserve the chemical signature of fractionation in these regions [3, 4]. Accurate measurements of the $N_2 + H_3^+$ reaction and its isotopologues require well-defined reactant internal energy distributions and collision energies. However, the H_3^+ ions produced in laboratory ion sources typically have elevated internal temperatures, often exceeding 1000 K, which can modify reaction cross sections and rate coefficients [5].

My research contributed to these infrastructure goals through three connected projects. I first diagnosed leaks in the external gas supply network, one in the line delivering gas to the ion source and another in the supply line feeding gas-dependent instrumentation. While these leaks did not compromise the vacuum envelope itself, they affected the delivery of gas essential for beam generation and instrument function. Resolving these issues ensured stable ion source operation and reliable instrument performance. I also updated an existing three-dimensional model of the apparatus in Autodesk Inventor to accurately reflect the configuration present in the laboratory. This update produced a reference model consistent with the as-built hardware, providing reliable documentation for future modifications and analysis. Finally, I performed Monte Carlo vacuum simulations in Molflow+ to predict pressure distributions and gas flow throughout the apparatus, allowing us to evaluate how design changes could influence experimental performance.

These projects, while focused on the engineering and operational aspects of the apparatus, had similar motivations as the reaction studies themselves, to enable reliable, reproducible laboratory data that can be directly applied to interpreting astronomical observations of cold molecular environments. By improving the integrity of gas delivery, mechanical documentation, and predictive modeling of the apparatus, this work supports the long-term goal of advancing our understanding of the chemical and physical evolution of interstellar gas from prestellar cores to protoplanetary disks.

In particular, reactions such as $N_2 + H_3^+ \rightarrow N_2H^+ + H_2$ and their isotopologues (e.g., N_2D^+) are chemically significant in prestellar cores, where they act as molecular tracers for dense, cold gas. Observations of the N_2H^+/N_2D^+ ratio allow astronomers to infer physical conditions, but these inferences require accurate laboratory cross-section data at low internal energies. The experimental setup simulates such conditions by merging fast beams of ions and neutrals with nearly co-propagating velocities, resulting in low relative kinetic energies comparable to those in cold astrophysical environments [8]. In the gas cell, a beam of N_2^+ is neutralized via charge exchange with cold N_2 gas before entering the interaction region. These experimental capabilities enable the controlled study of reactions crucial for astrochemical modeling.

2 Methods

My work focused on three main projects supporting the operation and long-term development of the merged fast-beams apparatus: diagnosing gas supply issues, updating the existing three-dimensional apparatus model, and simulating vacuum conditions. I completed each project to improve experimental stability and provide reliable documentation for future modifications.

2.1 Leak Detection

The first project involved identifying and addressing gas supply leaks affecting the ion source and laboratory instrumentation. The apparatus uses regulated gas flows to generate ion beams and operate instruments, including pressure gauges and pneumatic actuators.

2.1.1 Ion Source Gasline Leak

During experimentation, the deuterium gas supply feeding the ion source depleted much faster than expected. We temporarily replaced the deuterium feed with nitrogen to test the supply line and simplify diagnostics (Figure 2). Each gas line to the source was then independently isolated by closing downstream valves while monitoring pressure changes on two gauges, the nitrogen pressure gauge on the supply line and the turbo pump pressure gauge located near the ion source. For verification, nitrogen flow was applied until the Nitrogen gas regulator stabilized at 15 psi and the turbo pump gauge stabilized at approximately 1.10 * 10-5 Torr. Figure 3 shows the turbo pump gauge and Figure 4 shows the gauge on the Nitrogen gas regulator. The gas was stagnant in each section for 1 to 2 hours, and we checked the pressure to see if it had decreased significantly.

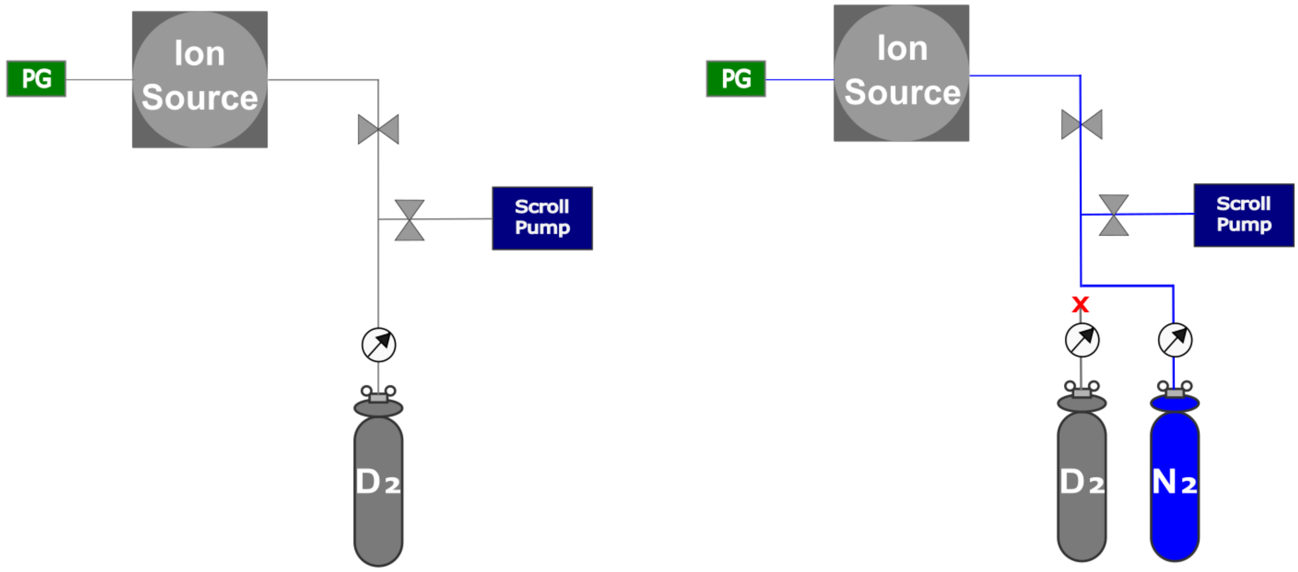

Figure 2: *Gas cylinder and supply line connections for deuterium (ion source feed) and nitrogen (instrument actuation).*

Figure 3: *Turbo pump pressure gauge used to monitor vacuum levels near the ion source during staged leak isolation diagnostics*

Figure 4: *Nitrogen gas regulator gauge used to isolate and test supply pressure to the ion source.*

2.1.2 Instrument Operation Gas Line Leak

The second leak affected the nitrogen supply used to operate pneumatic actuators for Faraday cups and gate valves. Since all four actuators failed simultaneously when pressure dropped, we concluded that the leak was likely located at the main connector feeding the control system (Figure 5). After resealing the connection, the actuator operation returned to normal.

Figure 5: *Main nitrogen connector suspected of leaking in the instrument control supply line.*

2.2 Schematic Updates

The second project focused on updating the apparatus's existing Autodesk Inventor model to accurately reflect its current configuration in the laboratory. The lab created the previous model before several modifications to object orientations (Figure 6), additions of flex bellows, and extensions added to the analysis region of the apparatus. Using reference drawings from component manufacturers, I revised the existing CAD assembly to incorporate these changes, ensuring that the model matches the as-built hardware. We used Autodesk Inventor Professional 2024 for these updates.

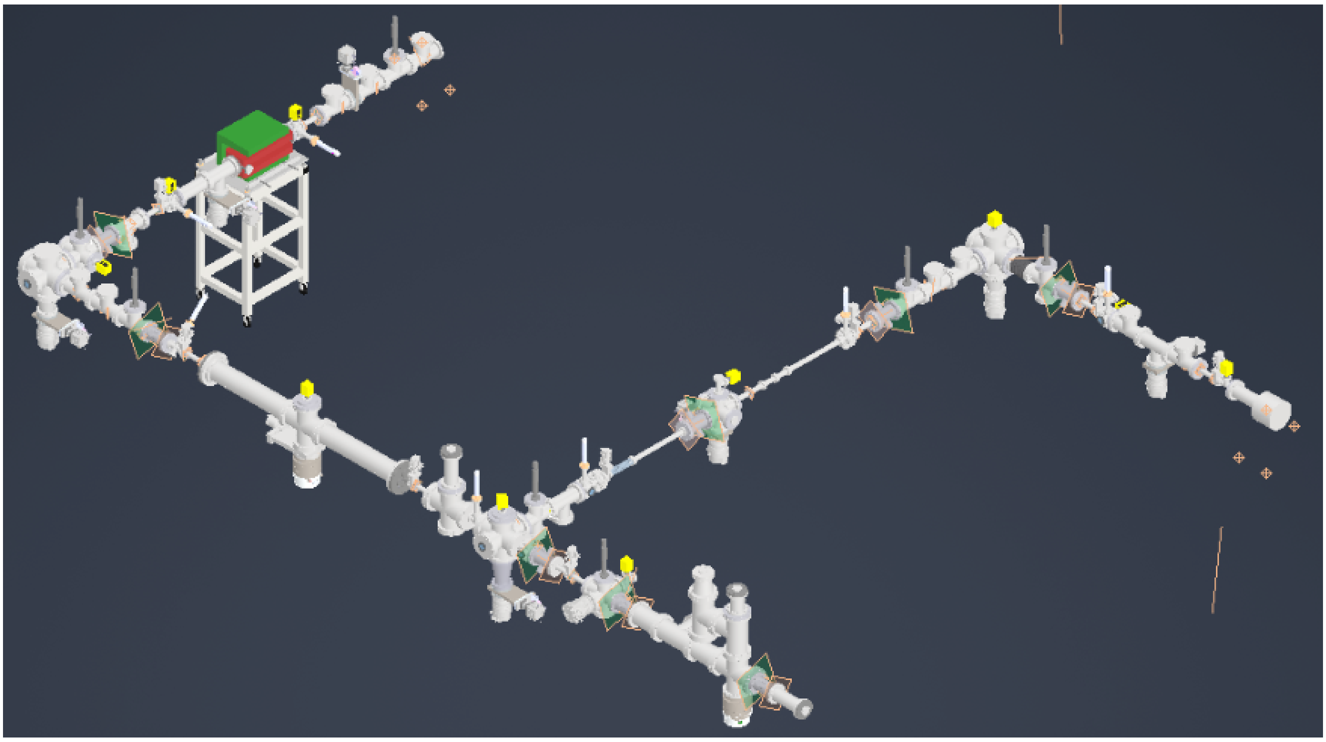

Figure 6: *Autodesk Inventor model of the Savin Group's apparatus from 2021.*

2.3 Vacuum Simulations

The third project focused on understanding how changes in apparatus geometry influence vacuum performance in regions critical for beam formation and reaction control. Well-characterized vacuum conditions are essential in merged-beams experiments to minimize background collisions and internal excitation of the reactant ions. To support this, I developed simplified models of the apparatus using Autodesk Inventor and performed Monte Carlo simulations in Molflow+ to evaluate gas flow and local pressure distribution.

My primary focus was the charge-to-mass filter (Wien filter) near the ion source, which had recently been modified by changing its exit aperture geometry. This region is important because it can influence the internal excitation of the H_3^+ beam prior to the interaction region. I modeled both the previous (closed) and updated (open) aperture designs in Inventor, exported the geometries as STL files, and imported them into Molflow+ for vacuum simulations.

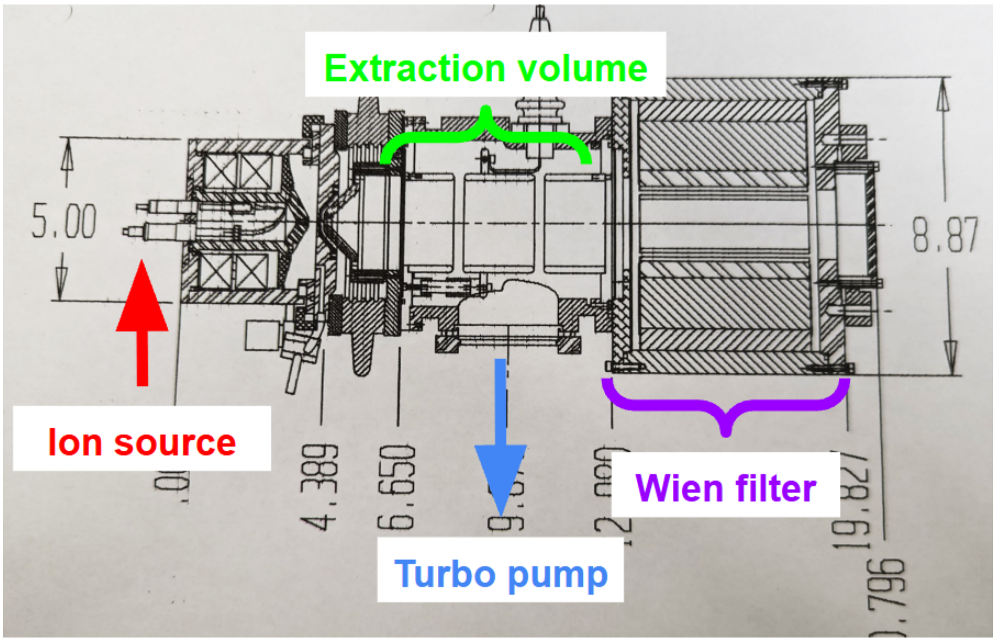

Figure 7: *The manufacturer schematic of the area being represented in vacuum simulations.*

3 Results

3.1 Leak Detection Results

3.1.1 Ion Source Gas Line Leak Results

The first leak was located somewhere within the deuterium gas supply system feeding the ion source. We expect that the leak originated in the deuterium gas regulator or one of its immediate connections (Figure 8). This conclusion is based on testing all other downstream connections and finding no leaks. However, we were unable to directly test the regulator itself because the deuterium cylinder had been depleted. As a result, the precise location of the leak within the regulator assembly remains uncertain.

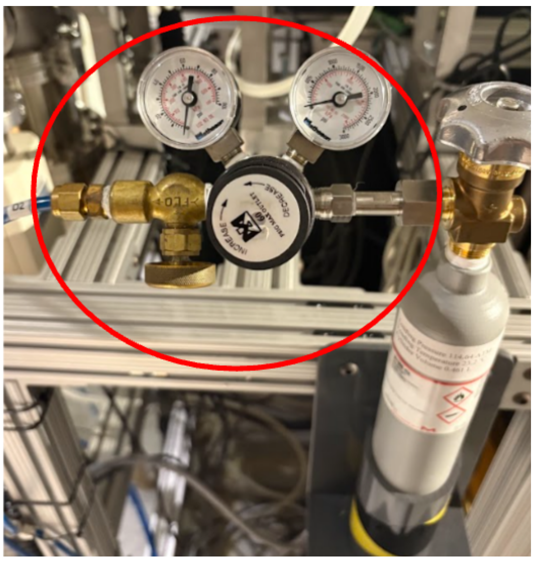

Figure 8: *Deuterium gas regulator and fittings suspected of contributing to the ion source feed leak.*

3.1.2 Instrument Operation Gas Line Leak Results

The second leak affected the nitrogen supply used to operate instrumentation such as the Faraday cup actuators. Since all four actuators lost gas supply and failed to respond properly, we concluded that the leak was likely located at the main connector feeding the control system or in the gas lines immediately downstream (Figure 9). After resealing the connector, actuator operation returned to normal and nitrogen consumption matched expected operating rates.

Figure 9: *Main nitrogen connector suspected of leaking in the instrument control supply line.*

3.2 Schematic Update Results

The existing Inventor model was updated to reflect these and other as-built changes to the apparatus. The updated model included a nipple extension added to the final analyzer (Figure 10), revised rotations for connections (Figure 11), and reoriented bellows assemblies (Figure 12). The resulting model now accurately represents the current hardware configuration and serves as a reliable basis for future apparatus modifications and documentation.

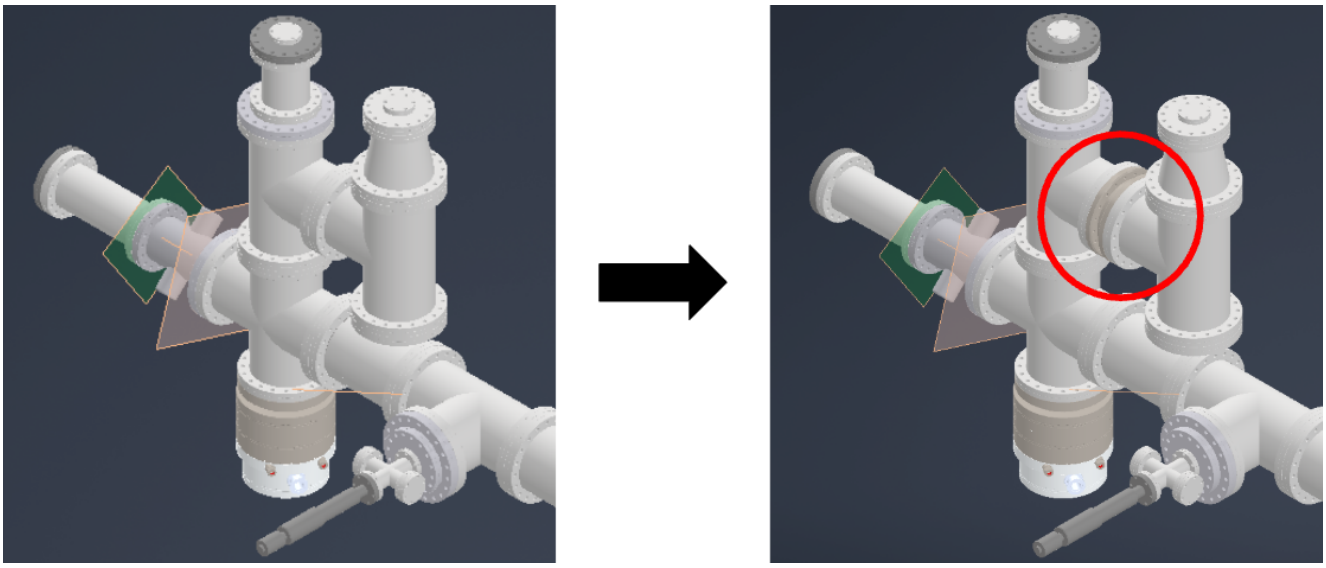

Figure 10: *Updated Inventor CAD model showing the nipple extension added to the final analyzer region. The left side is the old version, and the right side is the new version. The red circle indicates the changed area.*

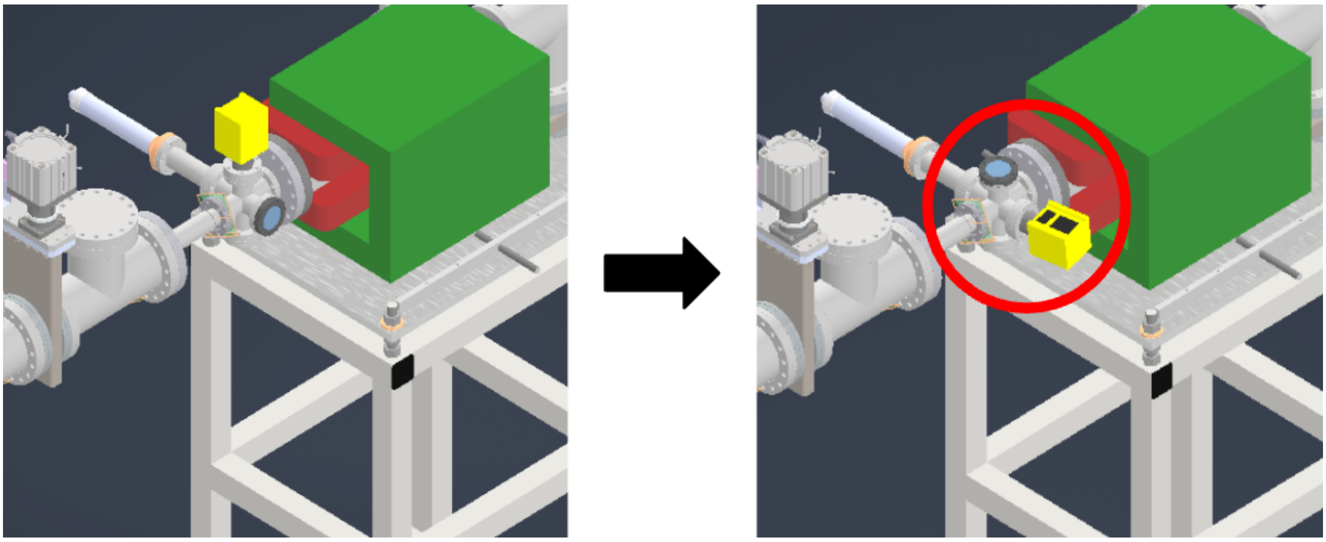

Figure 11: *CAD update showing revised component orientations. The left side is the old version, and the right side is the new version. The red circle indicates the changed area.*

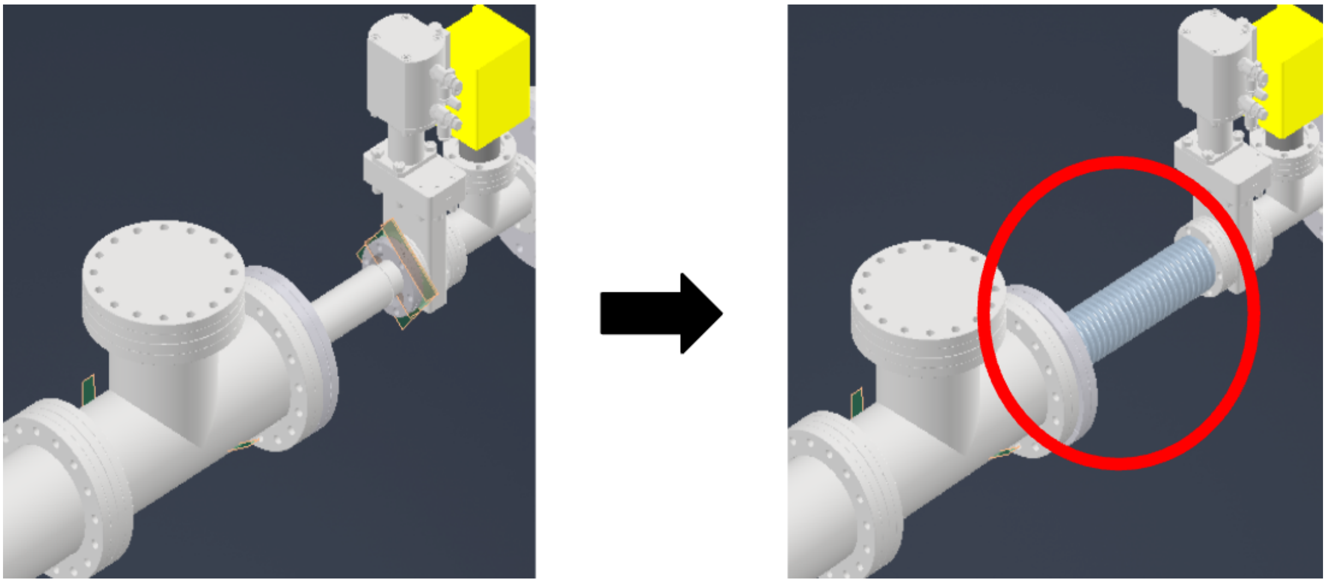

Figure 12: *CAD assembly showing added flexible bellows sections. The left side is the old version, and the right side is the new version. The red circle indicates the changed area.*

3.3 Vacuum Simulations Results

The vacuum simulations tracked the motion of hydrogen molecules from the gas inlet near the ion source to the turbo pump outlet. Using Molflow+, I ran Monte Carlo simulations for one hour of physical time to estimate the particle flux in the region of interest. For the open aperture geometry, the flux was approximately 1.89×10^{16} molecules $\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$, while the closed aperture geometry produced a flux of 5.70×10^{16} molecules $\mathrm{cm}^{-2}\ \mathrm{s}^{-1}$.

To convert these flux values into pressure estimates, I used relations from kinetic gas theory:

$$r = \frac{n\bar{v}}{4} \tag{1}$$

$$P = nk_BT \tag{2}$$

where r is the molecular flux, n is the particle density, $\bar{v}$ is the mean molecular speed, k_B is the Boltzmann constant, and T is the gas temperature.

Assuming $T = 300$ K and $\bar{v} \approx 1.49 \times 10^5$ cm/s for hydrogen at room temperature, the resulting pressure was 8.3×10^{-10} Torr for the open aperture and 4.2×10^{-9} Torr for the closed aperture. These pressures are both significantly below the typical baseline pressure of $\sim 10^{-5}$ Torr near the ion source. As shown in Table 1, the restrictive closed aperture results in approximately five times higher pressure in the excitation region compared to the open aperture.

Geometry	**Simulated Flux** (molecules/cm^2/s)	**Estimated Pressure** (Torr)
Closed aperture	5.70×10^{16}	4.2×10^{-9}
Open aperture	1.89×10^{16}	8.3×10^{-10}

Table 1: *Comparison of simulated gas flux and estimated pressure for different aperture geometries.*

While these results are preliminary, they provide valuable insight into how small geometric modifications—such as a 1 mm aperture change—can significantly influence local vacuum conditions. A fivefold increase in pressure could increase the probability of collisions that re-excite ions after their formation in the source, potentially affecting reaction cross sections and product yields.

This work represents the first application of Molflow+ on this apparatus. The simulations assumed ideal pumping conditions and estimated gas flow rates, which will be refined in future modeling efforts. Follow-up simulations will incorporate detailed conductance values and measured flow rates to better match experimental conditions. These findings have already informed ongoing design discussions, and Dr. Ivanov is using the flux-based pressure estimates to evaluate the impact of geometry on source performance and internal excitation control.

4 Conclusions

This project supported the operation and development of the dual-source merged fast-beams apparatus by improving gas supply reliability, updating mechanical documentation, and establishing a foundation for vacuum performance modeling. Two external gas supply leaks were identified and addressed, one in the deuterium feed to the ion source and another in the nitrogen supply for instruments such as the Faraday cups and gate valves. These repairs stabilized gas delivery and improved the reliability of beam generation and instrument operation. The existing three-dimensional Inventor model of the apparatus was updated to accurately reflect the configuration in the lab, providing a reliable reference for future design modifications. Preliminary vacuum simulations using Molflow+ demonstrated how geometric features and pump configurations affect vacuum performance, establishing a path toward more comprehensive modeling.

Through these activities, I gained practical skills in CAD modeling for experimental design, gas line leak diagnostics, and vacuum simulation techniques. More broadly, this work reinforced the importance of detailed documentation and systematic troubleshooting in experimental research, showing how even small physical changes can significantly influence experimental performance.

The accurate measurement of ion-neutral reaction cross sections depends on stable and reproducible experimental conditions. By addressing gas supply issues and improving apparatus documentation, this work enhanced system reliability and created tools for evaluating and predicting pressure behavior. Together, these efforts strengthen the experimental foundation for high-precision studies of reactions such as $N_2 + H_3^+$, improving the astrophysical relevance of laboratory data.

Future work could extend the vacuum simulations to incorporate updated geometries for additional parts of the apparatus and compare simulated pressure profiles with experimental measurements to validate model accuracy. These continued efforts will further improve experimental reliability and enhance the laboratory's capability to conduct precision measurements of astrochemically important ion-neutral reactions.

Future simulation work will also examine other geometry modifications, such as baffle structures or aperture tuning, and evaluate their influence on beam purity and internal energy. Comparing simulated pressure profiles to experimental gauge readings will provide validation and guide optimization of beamline performance for astrochemical experiments.

5 Acknowledgements

This material is based upon work supported by the National Science Foundation under Grant No. PHY-2349438.

References

[1] T.J. Millar. Deuterium fractionation in interstellar clouds. *Planetary and Space Science*, 51(2):119–124, 2003.

[2] O. Sipilä, E. Hugo, J. Harju, O. Asvany, M. Juvela, and S. Schlemmer. Modelling line emission of deuterated h3+ from prestellar cores. *Astronomy & Astrophysics*, 509:A98, 2010.

[3] A. Crapsi, P. Caselli, C.M. Walmsley, P.C Myers, M. Tafalla, C.W. Lee, and T.L. Bourke. Probing the evolutionary status of starless cores through n_2h^+ and n_2d^+ observations. *The Astrophysical Journal*, 619(1):379–406, 2005.

[4] E. Redaelli, L. Bizzocchi, P. Caselli, O. Sipilä, V. Lattanzi, B. M. Giuliano, and S. Spezzano. High-sensitivity maps of molecular ions in l1544. i. deuteration of $\mathrm{n_2h^+}$ and $\mathrm{hco^+}$ and primary evidence of $\mathrm{n_2d^+}$ depletion. *Astronomy & Astrophysics*, 629:A15, 2019.

[5] D. Gerlich and S. Schlemmer. Deuterium fractionation in gas-phase reactions measured in the laboratory. *Planetary and Space Science*, 50(12):1287–1297, 2002. Special issue on Deuterium in the Universe.

[6] A. P. O'Connor, Urbain X., J. Stützel, K. A. Miller, N. De Ruette, M. Garrido, and D. W. Savin. Reaction studies of neutral atomic C with $\mathrm{H_3^+}$ using a merged-beam apparatus. *The Astrophysical Journal Supplement Series*, 219(6), 2015.

[7] D. W. Savin, A. P. O'Connor, O. Novotný, X. Urbain, J. Stützel, and ... Reaction studies of neutral atomic c with $\mathrm{h_3^+}$ using a merged-beams apparatus. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 53(1):015201, 2020.

[8] H. Bruhns, H. Kreckel, M. Lestinsky, B. Seredyuk, W. Mitthumsiri, B. L. Schmitt, M. Schnell, X. Urbain, M. L. Rappaport, C. C. Havener, and D. W. Savin. A novel merged beams apparatus to study anion-neutral reactions. *Review of Scientific Instruments*, 81(1), 2010.