National Aeronautics and Space Administration

FY23 Strategic Initiatives Research and Technology Development (SRTD)

Cosmic Origins of Earth's Oceans

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Strategic Focus Area: The Science of Water in the Universe | **Strategic Initiative Leader:** Leonidas A Moustakas

Objectives: To improve our understanding of the distribution and isotopic composition of water in the Solar System by developing new modeling tools and carrying out laboratory experiments to interpret isotopic ratio measurements, which in turn will drive future missions.

Background:

A statistical study comparing the isotopic composition of different comet reservoirs (Oort cloud vs. Kuiper belt) with the Asteroid belt is needed to test Solar System formation models combining chemistry and dynamics. For future space missions (e.g., the JPL Astrophysics Probe, PRIMA), modeling uncertainties will become a limiting factor. The state-to-state collisional cross-sections are only available for $H_2{}^{16}O$ on $H_2{}^{16}O$. The collisions for other isotopologues are expected to be different, affecting the accuracy of the isotopic ratio measurements. Moreover, good understanding of fractionation processes during water sublimation from ices is required to ensure that the isotopic ratios in the coma are representative of the bulk composition of the nucleus.

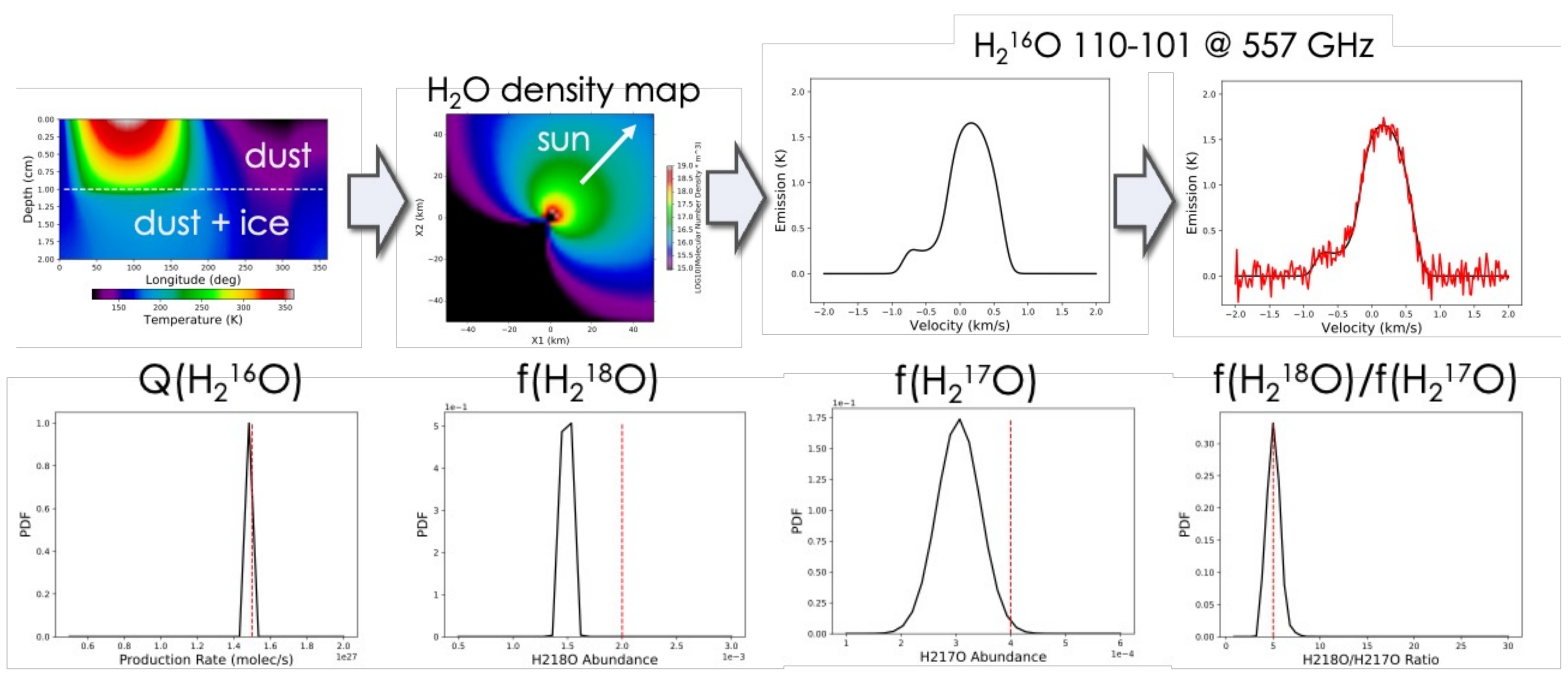

Figure 1. (Top) Steps for producing synthetic spectra of molecular emission lines. (Bottom) The posterior probability distributions for the water production rate and the isotope abundances (from publication [A]).

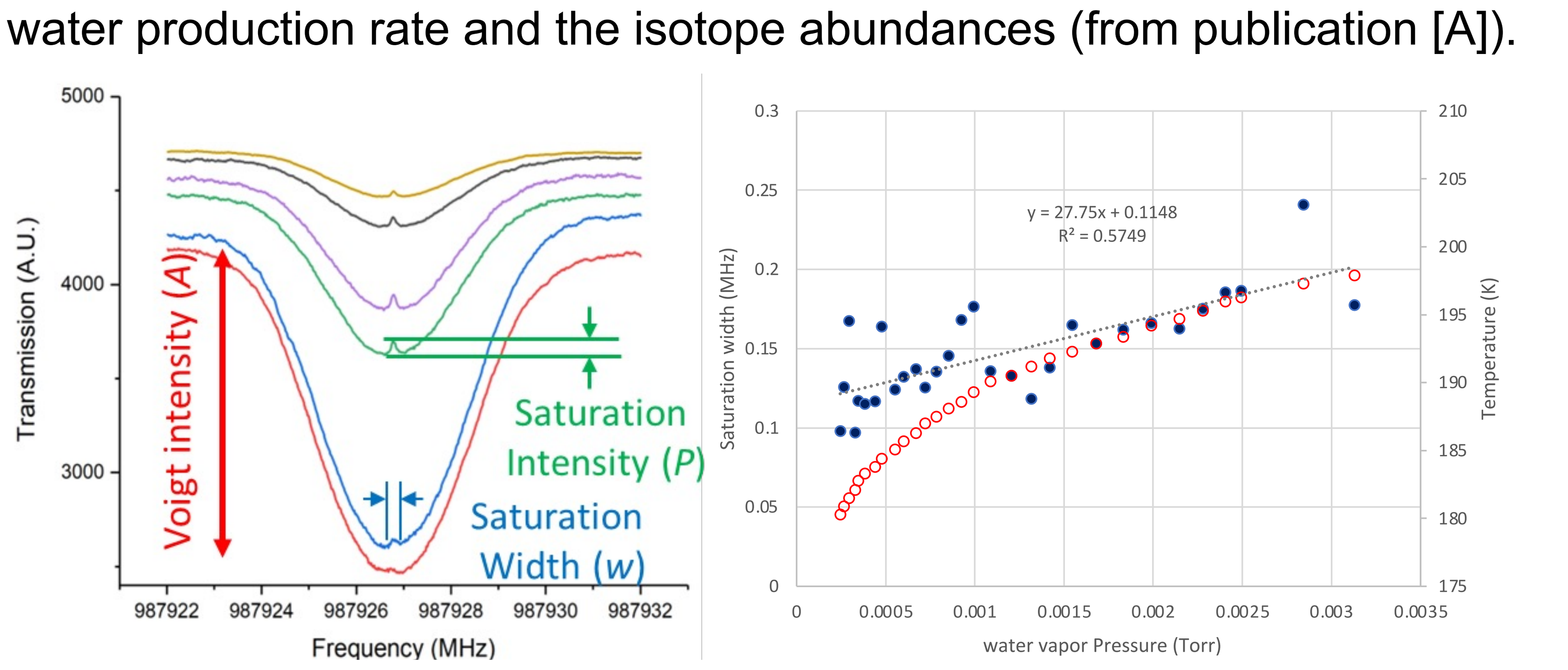

Figure 2. (Left) Absorption profiles at different water vapor pressures showing saturation 'dip' features with measurable pressure dependences even at exospheric vapor pressure levels. (Right) Initial low pressure saturation data (solid blue circles) set recorded sample volatility limited by cell temperature that was slowly drifting (open red circles).

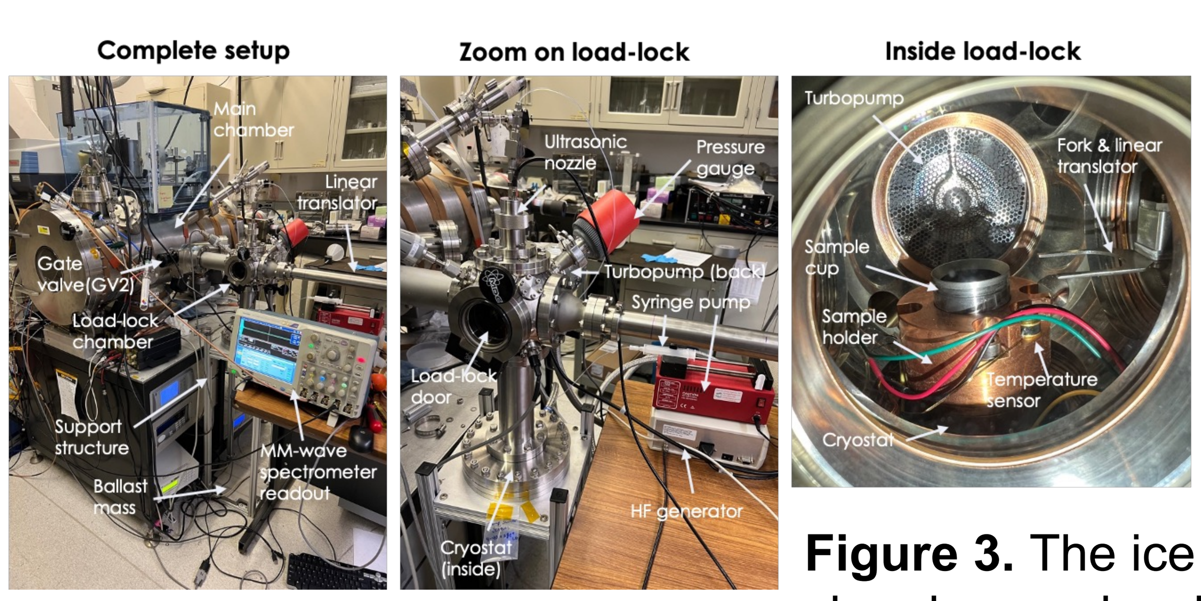

Figure 3. The ice sublimation chamber as developed in this project.

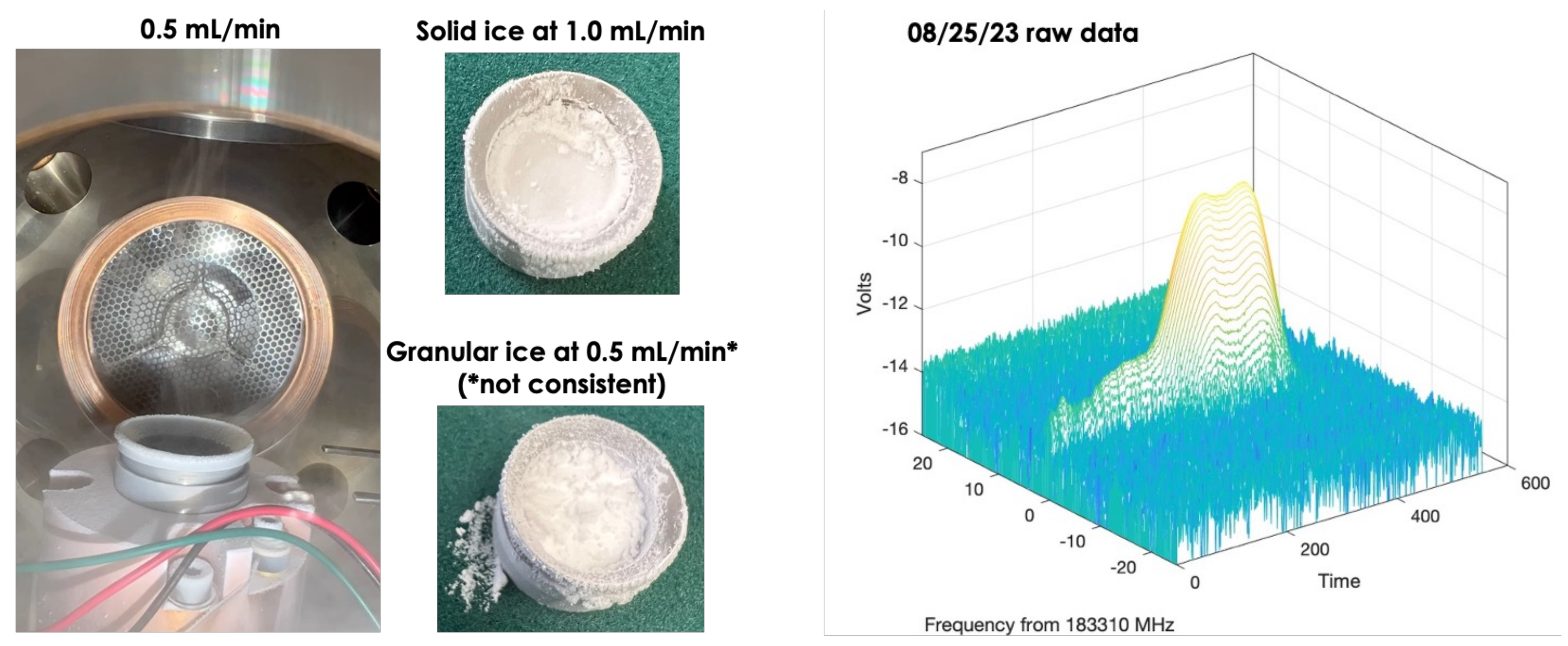

Figure 3. (Left) Ice samples being prepared and their aspects at water flow rates of 0.5 mL/min and1 mL/min, after extraction from the load-lock chamber after preparation. (Right) Time-ordered mm-wave spectra in integer number of spectra acquired during a complete sublimation run. Note the increase in line amplitude and area, before decrease and disappearance as pressure kept increasing above 10^{-2} torr.

Approach and Results:

Task 1 – Modeling the structure of comae.

A key innovation is that the physical parameters of the nucleus subsurface region determine the computed line intensities with no empirical parameters. Figure 1 (upper panel). We established that the intensity of the water emission is primarily determined by the dust thickness rather than the ice content. We established that the $H_2{}^{18}O$ to $H_2{}^{17}O$ abundance ratio can be retrieved from synthetic observations with the high accuracy needed to advance our understanding of isotopic fractionation in the early Solar System (Figure 1, lower panel).

Task 2 – Molecular collisions.

A collisional cooling apparatus was refurbished and shown to be useful for saturation spectroscopy at 170–300K. Analysis of saturation spectroscopic measurements (Figure 2) at 190–210 K and 300 K suggests a regular power law dependence of broadening. A mixed H_2O and HDO sample was introduced repeatedly until the cell was completely passivated with partially deuterated water. Low temperature measurements of the 987 GHz H_2O line indicate reduced collisional broadening, despite the obvious quenching of the saturation feature.

Task 3 – Lab measurements of water sublimation from solid surfaces

We upgraded a cryogenic vacuum chamber with the capability to prepare water ice samples in-situ (Figure 3). Samples are prepared inside the load-lock by ultrasonic atomization of liquid water at 130 kHz and microdroplets deposited into a sample cup pre-cooled under high vacuum (Figure 4, left). The sample cup is transferred under vacuum into the main chamber, where it is slowly heated from 125 to 260 K. Total vapor pressure is continuously measured via pressure gauges, and the water lines surveyed using the mm-wave spectrometer. $H_2{}^{16}O$ and HDO sublimation experiments have been completed using vapor-deposited ice samples, and preliminary sublimation experiments of ice samples conducted with H_2O line survey (Figure 5, right).

Significance/Benefits to JPL and NASA:

Our theoretical models and laboratory experiments guide formulation of future planetary and astrophysics space missions, such as PRIMA or WISPER, a smallsat concept for a flyby of a nearby comet,

Our work also leads to follow-up theoretical, experimental, or technical ROSES proposals. Related funded tasks include PICASSO and APRA tasks. A new collaboration with the University of Wisconsin-Madison includes student exchange, NSF and SSW proposals in preparation, joint publications and observing proposals (NOEMA and JWST).

Publications: [A] P. von Allmen, et al., *Retrieval of water isotopologue abundance from microwave observations of a cometary coma.* A&A, in prep, (2023). [C] W.E. Thompson, et al., *Comparing Complex Chemistry in Neighboring Hot Cores: NOEMA Studies of W3(H2O) and W3(OH).* Ap. J., 952, 50(2023). [D] N. Biver, et al., *Coma composition of comet 67P/Chuyumov-Gerasimenko from radio-wave spectroscopy.* A&A, 672, A170 (2023/04). [L] N.X. Roth, et al., *Leveraging the ALMA Atacama Compact Array for Cometary Science: An Interferometric Survey of Comet C/2015 ER61 (PanSTARRS) and Evidence for a Distributed Source of Carbon Monosulfide.* Ap.J., 921, 14 (2021/11). [M] N. Biver, et al., *Molecular composition of short-period comets from millimetre-wave spectroscopy: 21P/Giacobini-Zinner, 38P/Stephan-Oterma, 41P/Tuttle-Giacobini-Kresák and 64P/Swift-Gehrels.* A&A, 651, A25 (2021/07).

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