National Aeronautics and Space Administration

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: The overarching goal is to improve our understanding of the distribution and isotopic composition of water in the Solar System by developing improved modeling tools and carrying out laboratory experiments needed to interpret isotopic ratio measurements, which in turn will drive future missions. Measurements of the D/H ratio in water provide important constraints on the origin and history of water molecules, and the contribution of comet-like bodies to Earth's oceans. A statistical study comparing the isotopic composition of the Oort cloud and Kuiper belt with that of the Asteroid belt is needed to test Solar System formation models combining chemistry and dynamics.

Background: Isotopic composition of the inner Solar System (Asteroid belt) is relatively well determined from the 100+ measurements in meteorites. Comets are the best tracers of the isotopic composition of the present day outer Solar System, because they have atmospheres and can be studied using remote sensing techniques. As underlined in the latest Planetary Science Decadal Survey, D/H variations are large, a factor of 3. Therefore, the required accuracy of individual measurements is much more forgiving than for other isotopic ratios. However, only 4 accurate D/H measurements have been taken over the past 25 years. The work carried out in this task will lead to significant improvements in the accuracy of future isotopic ratio measurements through (1) Development and implementation of improved coma excitation models; (2) Calculation and experimental verification of water-water and water-heavy water collision rates; and (3) Detailed parameterization of water and heavy water vaporization processes at low temperatures, which may affect isotopic ratios in the gas phase.

Approach and Results:

Task 1 – Modeling the structure of comae and exospheres. We have developed a numerical code to compute the profiles in a non-spherical coma, including collisions and non-gravitational forces, using the physical properties of the nucleus sub-surface as input parameters to the model. We validated our model by comparing computed water vapor emission lines with results from the literature. We used a Bayesian approach for uncertainty quantification to understand the sensitivity of the water vapor emission lines to model parameters (Figure 1).

Task 2 – Molecular collisions. The JPL collisional cooling apparatus is being used to examine the effects of collisions on molecular line shapes, and these effects will be quantitatively compared with the predictions of calculations. Spectra have been recorded at 170-300 K for both 556 GHz (1-1) and 987 (2-1) GHz transitions of H_2O. Cryogenic system has been shown to be capable of measurement of water saturation vapor pressures down to 170 K.

Task 3 Water sublimation from solid surfaces – Laboratory measurements. The modular FTmmW system has been shown to measure H_2O and HDO at pressures of a few microtorrs, making the sensitivity adequate for measurements below 180K. We mitigated chamber operational issues that prevented establishing a high enough vapor pressure within the chamber from sublimated ice by adding heater elements to the cryostat. We developed an ultrasonic atomization system that will allow to prepare granular ice of controlled and reproducible grain size and characterized the grain size distribution via cryogenic optical microscopy (Figure 2). We integrated the ultrasonic atomization system with the vacuum chamber and are finalizing integration of the cryostat to prepare ice directly within the load-lock. We conducted preliminary measurements of water vapor pressure over vapor-deposited ice.

Significance/Benefits to JPL and NASA: Theoretical models and laboratory experiments will guide formulation of future planetary and astrophysics space missions. PRIMA is a FIR Astrophysics Probe concept currently in formulation at 7X. This 2-m class cryogenically cooled telescope equipped with a medium-resolution direct detection spectrometer would measure D/H in ~50 comets in a nominal 5-year mission. WISPER, a smallsat mission concept for a flyby of a nearby hyperactive comet using a passively cooled Schottky instrument, has been studied by 4X as a possible SIMPLEx 3 candidate. Source, a 3-m diameter passively cooled FIR telescope with a cryogenically cooled SIS heterodyne spectrometer was studied by 7X as a MIDEX candidate. The concept was priced above the MIDEX cost cap and is being re-scoped and optimized for the next MIDEX AO to provide maximum synergies with PRIMA.

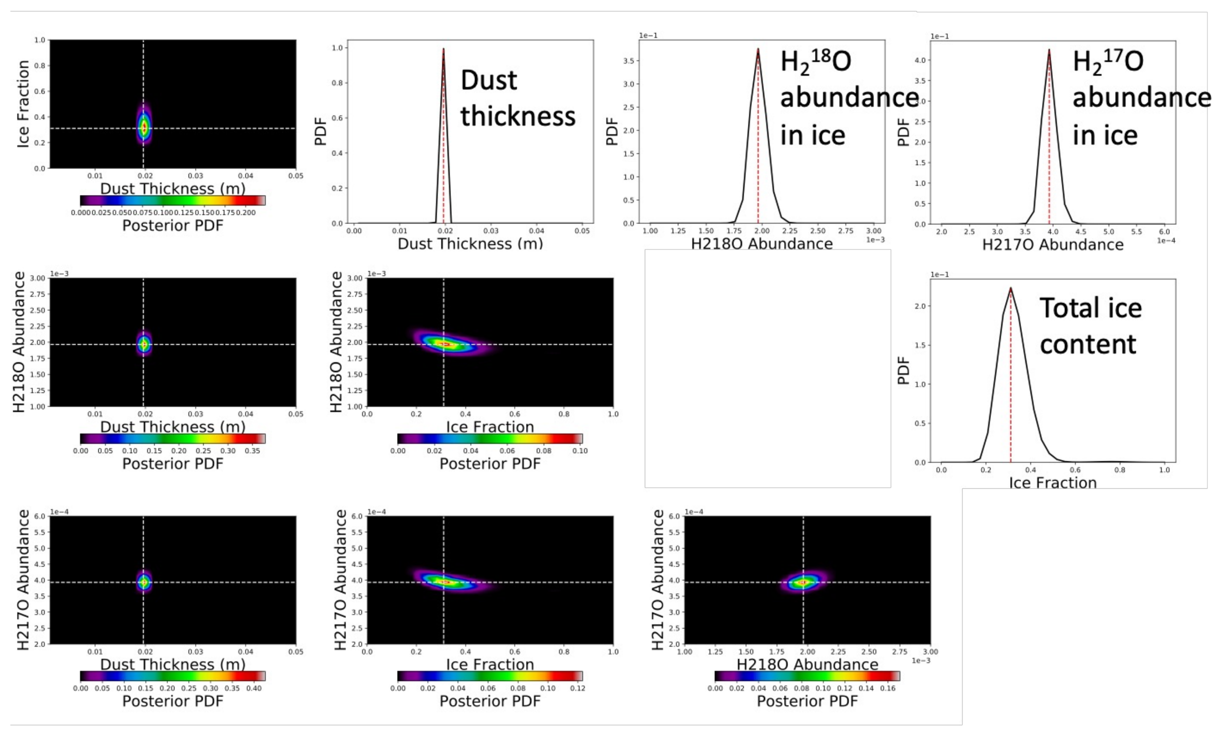

Figure 1. Posterior Probability Distribution Functions for nucleus model parameter retrieval from synthetic $H_2^{16}O$, $H_2^{17}O$, and $H_2^{18}O$ emission lines. Model parameters are applicable to a smallsat flyby: observer range 5000 km, heliocentric distance 1.9 au.

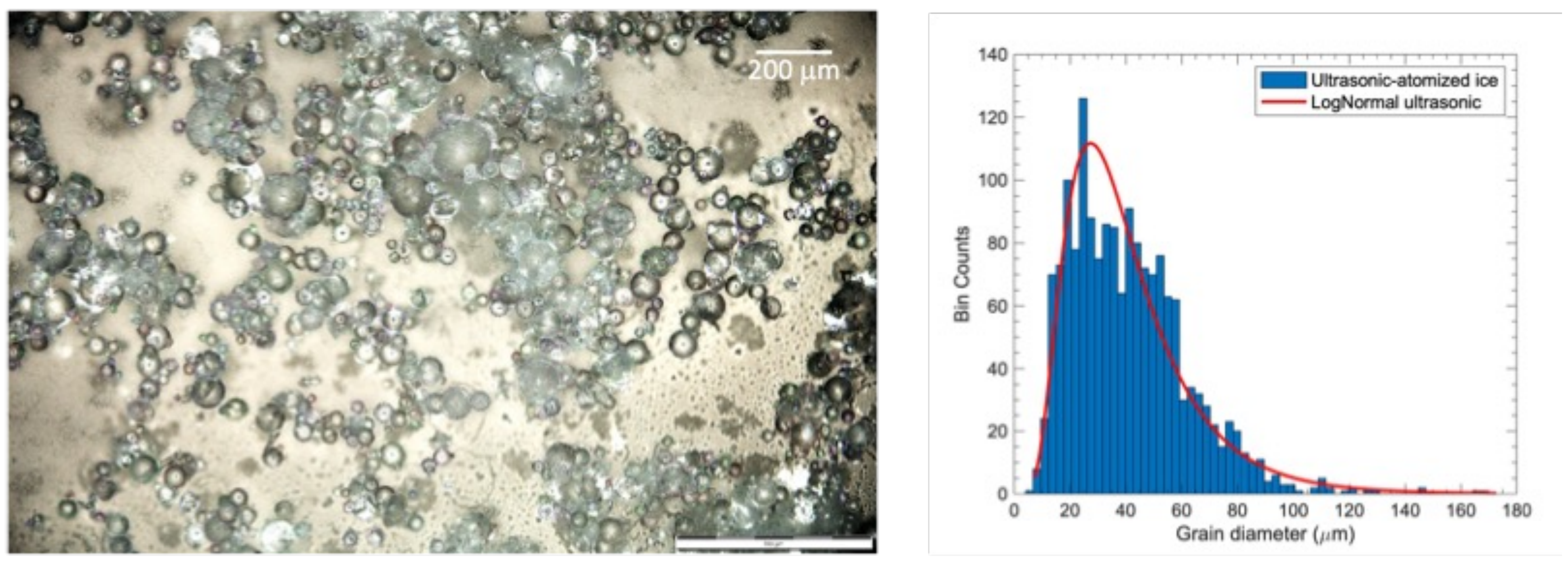

Figure 2. (Left) Ice sample prepared using the ultrasonic atomization system (-100°C within Linkam LTS350 cryostage) imaged with Olympus BX51 microscope under reflected illumination using extended focal imaging. (Right) Resulting grain size distribution follows a log-normal distribution, expected for pulverization/atomization of materials, and also observed in air atomized ice.

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Publications (FY22):

N. Biver, D. Bockelée-Morvan, J. Crovisier, R. Moreno, J. Boissier, G. Paubert, S. Milam, D.C. Lis, et al., *Did we see the same comet 67P/Churyumov-Gerasimenko in 2021 as Rosetta?* Poster, Annual Planetary Science Meeting, Lyon, France (2022/06).
B. Drouin, D.J. Nemchick, T.J. Crawford, P. von Allmen, and D. Lis, *Measurement of Collisional Self-Broadening at Low-Temperatures using Sub-Doppler Spectroscopy.* Int. Symp. Mol. Spec, Urbana-Champaign, IL (2022/06).
W.E. Thompson, S.L. Widicus Weaver, and D. Lis, *NOEMA Observations of Complex Organic Chemistry in the W3 Star-Forming Region.* Int. Symp.on Mol. Spec., Urbana-Champaign, IL (2022/06).

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