National Aeronautics and Space Administration

FY23 Strategic Initiatives Research and Technology Development (SRTD)

Water Formation and Heritage Across Cosmic Time

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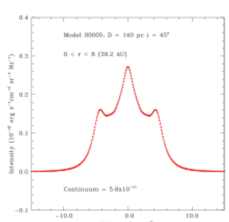
Strategic Focus Area: The Science of Water in the Universe **| Strategic Initiative Leader:** Leonidas A Moustakas

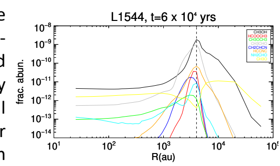
Objectives: To investigate the links between water and related molecules during the star and planet formation process. **Task 1:** Investigate excitation and radiative transfer in the HD molecule, in order to understand its utility as tracer of disk mass. **Task 2**. Study how water and complex organic molecules (COMs) form in ices in molecular clouds and disks. **Task 3.** Study how water is distributed and how it migrates in protoplanetary disks to understand how water ends up in the planets, small bodies (comets, asteroids) and dust in planetary systems by carrying out state-of-the-art chemical and dynamical modeling. **Task 4.** Determine how the current value of the deuterium-to-hydrogen (D/H) ratio of Uranus and Neptune is reproduced by solid accretion taking place during the process of forming, using both analytical and numerical approaches. **Task 5.** Determine if polarization can be used to differentiate water clouds from sulfuric acid clouds, and if acid concentration is low enough to support life as we know it on an exo-Venus to be discovered using a future 6-m space telescope with a starshade.

Approach and Results:

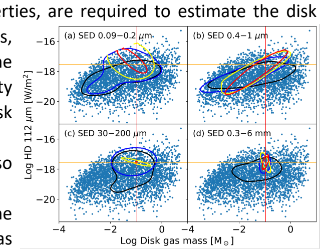
Task 1: We analyzed the HD emission from a range of ProDiMo models. Shown is the HD J=1-0 spectrum from the central region of a 0.036 M_{sun} mass protoplanetary disk around a 1.8 M_{sun} star. Disks have cold midplanes and hot, flared surfaces, yielding large temperature gradients that result in complex line profiles when the HD optical depth is appreciable, which occurs in higher mass disks. The finite optical depth also results in HD emission from portions of the disk and in consequence the total flux being reduced, thus giving an incorrectly low value of the HD abundance (and consequently) the disk mass.



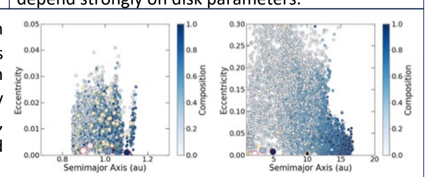
Task 2: We have completed models of COMs and water chemistry in several well studied prestellar cores. Trends in the formation of COMs with density and temperature have been determined, and model predictions compared to observations. The figure shows results for L1544, where observations have been made towards the core center and towards the methanol peak (4000au from center, shown by dashed line). The models provide good fits to the observations at both peaks, with the methanol peak appearing to be slightly chemically younger than the core center.



Task 3: We modeled 3000 disks with time-dependent chemistry and radiative transfer processes using the ProDiMo code. We found that at least three physical parameters, the central star, disk size, and dust properties, are required to estimate the disk gas mass, which is the key quantity driving disk dynamics. We can also accurately estimate the disk gas mass using the far-IR or submm SED (see figure). We also found that the water mass in disks is dominated by the ice. and the total water abundance does not depend strongly on disk parameters.



Task 4: To study the accretion of solids on to forming planets we have used a state-of-the art N-body code in which the dynamics of solids with a wide size range (~ 1m to >10^3 km) is reliably computed. This capability is critical as we are interested in reliably tracing how (proto)Uranus undergoes deuterium enrichment through solid accretion. Shown are two examples of simulation results. By coupling simulation results with chemistry models in a post-processing fashion, we can compute the composition of planets. As an example, a spatially, linear distribution of water is considered in the plot. We confirm that global simulations are crucial as a good amount of mixing of water could occur during planet formation processes.

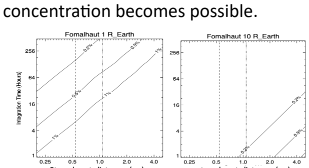


Significance/Benefits to JPL and NASA:

Our results are relevant to current and future JPL missions

- We have demonstrated that HD emission is a useful tracer for measuring disk gas mass supporting one of the science goals of the PRIMA mission concept
- We show that velocity resolved spectroscopy and spatially resolved imaging of the HD emission from protostellar disks will be hugely valuable for determining the HD and mass distribution and should be pursued for future missions.
- The recently released decadal strategy for planetary science and astrobiology recommended Uranus orbiter and probe (UOP) as a next flagship mission at the highest priority. The research conducted is directly relevant to this recommendation, and hence puts JPL at a stronger position to lead the mission.
- JWST is capable of detecting COMs in ices. Our results will support proposal submission and the interpretation of data.

Task 5: We calculated polarization models for an exo-Venus and found that for a noise level of 1% or better in the planetary flux differentiation of water and acid, and retrieval of acid concentration becomes possible.



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Publications:

Hasegawa (2022) *Solid Accretion onto Neptune-mass Planets. I. In Situ Accretion and Constraints from the Metallicity of Uranus and Neptune* ApJ, 935, 101
West, R. et al. (2022) *Spectropolarimetry as a means to address cloud composition and habitability for a cloudy exoplanetary atmosphere in the habitable zone*, ApJ, 940, 183

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