Modeling the Chemistry and Spectra of Water World Atmospheres with PICASO

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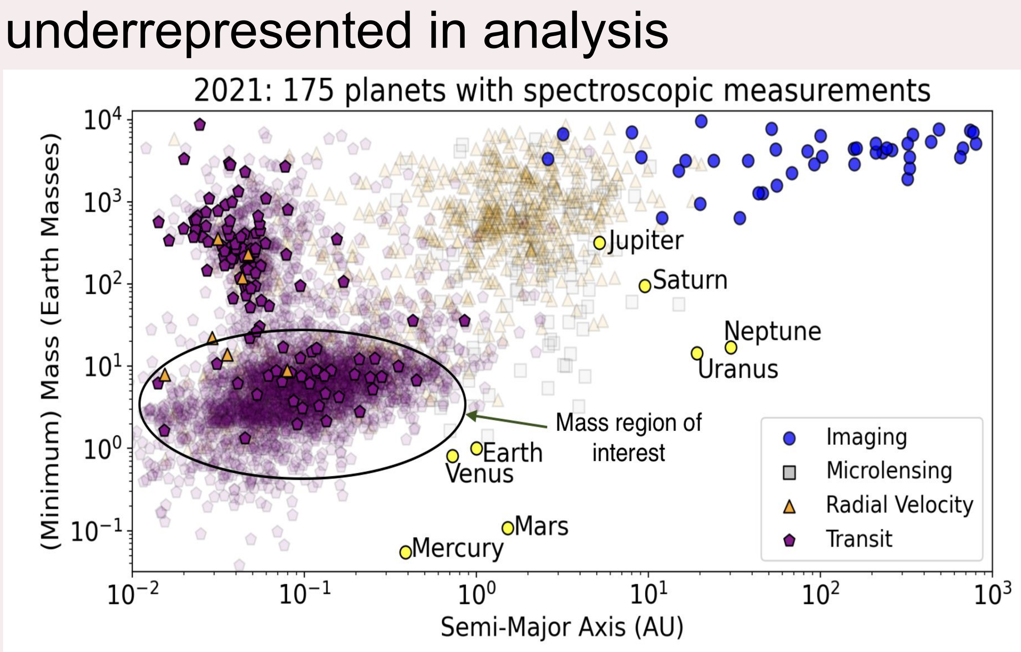
Abstract

So far, the quantitative study of **water world atmospheres** has lagged far behind the study of giant planets, sub-Neptunes, and terrestrial planets, which we aim to rectify. Here, we investigate water worlds' time evolving **atmospheric chemistry,** coupled to planetary cooling, mediated by the important and changing interface between a water layer and the magmatic rocky layer beneath. We use these chemistry calculations and corresponding fully coupled 1D radiative-convective atmospheric structure calculations to model spectral diagnostics of main atmospheric absorbers. A goal is to understand important absorbers beyond steam, which may be diagnostics of atmospheric and **atmosphere/mantle interface conditions**. This work enhances the capabilities of the open-source atmosphere modeling code **PICASO** to include atmospheres not dominated by H/He.

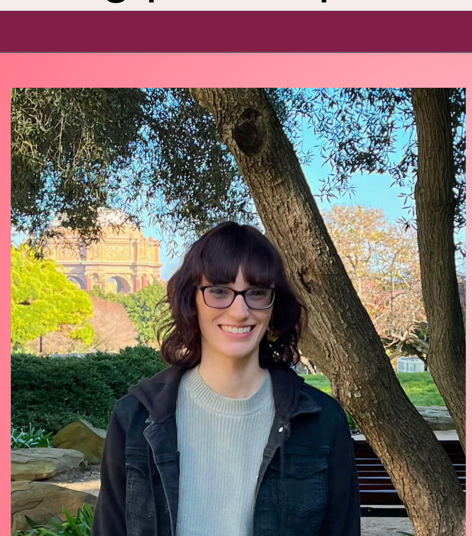
Why We Need to Create Models for Water World Atmospheres

With the launch of JWST, we are now able to better study smaller planets, but they are still underrepresented in analysis



Graph of exoplanets as of 2021 that have spectroscopic measurements. Smaller, rocky planets make up the majority, but are understudied. Image adapted from Dmitry Savransky with data from NASA Exoplanet Archive

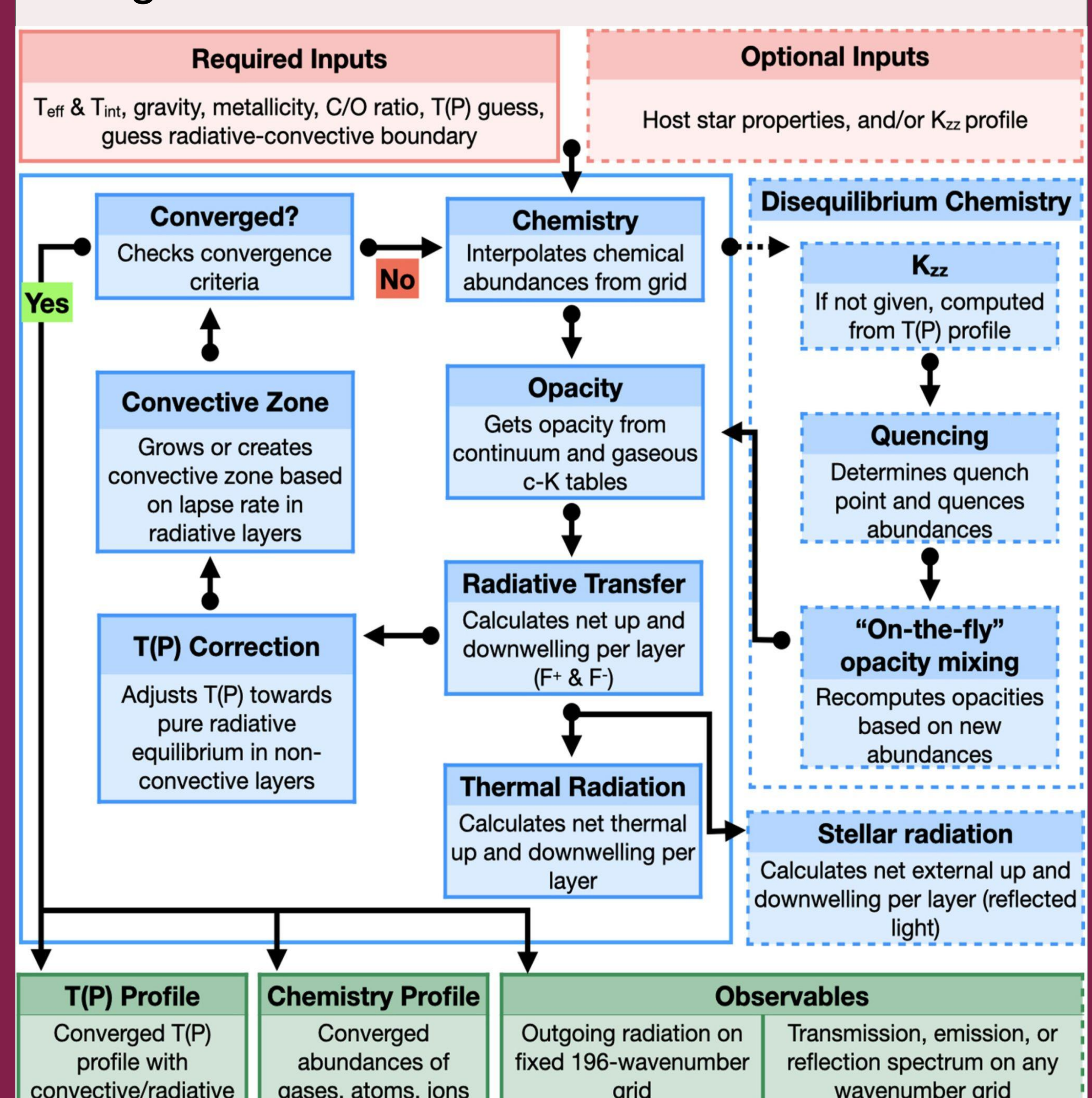
We can study the atmospheres of these planets through retrievals (allowing each atmosphere parameter to vary freely until one achieves a best fit model) or grid-retrievals (creating a grid of radiative-equilibrium models over a range of parameters and performing analysis on them). Grids can be modeled with **PICASO** using precomputed chemistries.



Scan to learn more about PICASO!

The PICASO Climate Model

- **PICASO** is a python-based open source atmospheric model with its legacy from the **EGP** model. It was developed and optimized to model the atmospheres of H_2/He rich atmospheres, and has been used to model transiting gas giants, directly imaged planets, and brown dwarfs.
- What **PICASO** can do:
  - Create 1D radiative-convective thermochemical equilibrium models
  - Model disequilibrium chemistry self-consistently
- The user can perform further analysis on the models by:
  - Adding clouds in post-processing
  - Using another code to perform a grid-retrieval on the models



Schematic of the workflow of PICASO from Mukherjee et al 2023 ApJ 942 71

- How **PICASO** works:
  - Inputs:
    - Stellar and planetary parameters
    - Initial guesses for the T(P) profile and the radiative-convective boundary
    - Atmospheric metallicity and C/O ratio
  - Outputs:
    - A converged T(P) profile
    - Chemical abundances
    - Spectra – transmission, thermal emission, and reflection

Contact us if you have questions!

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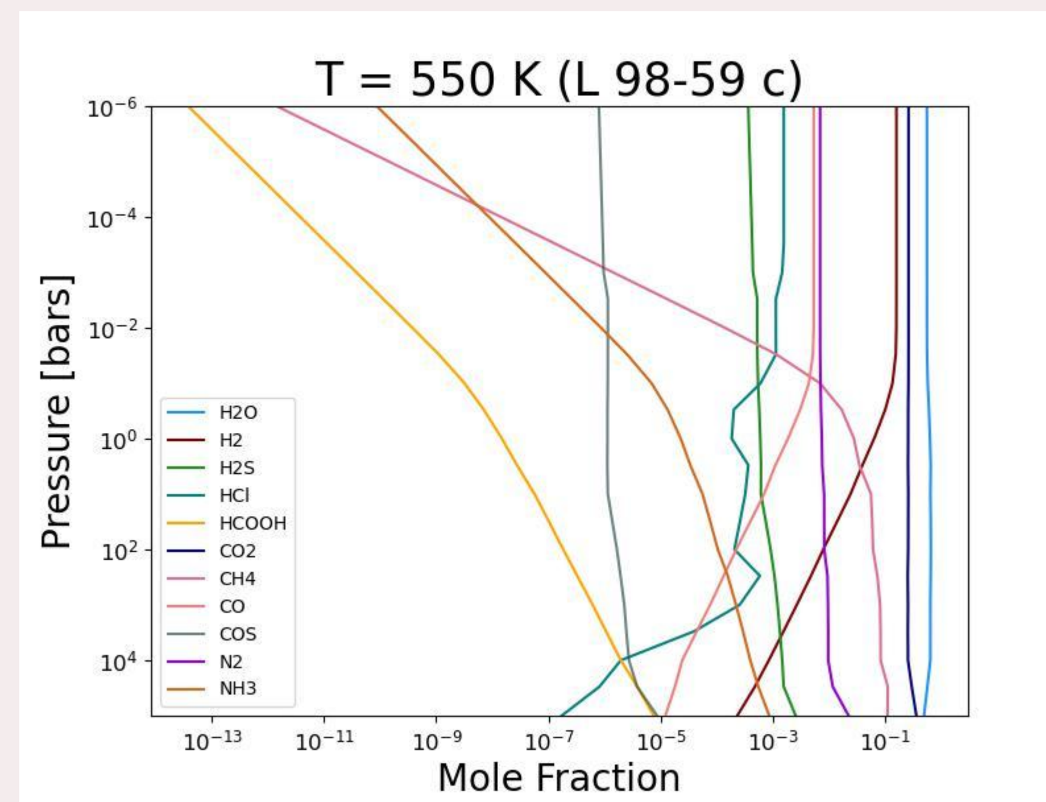
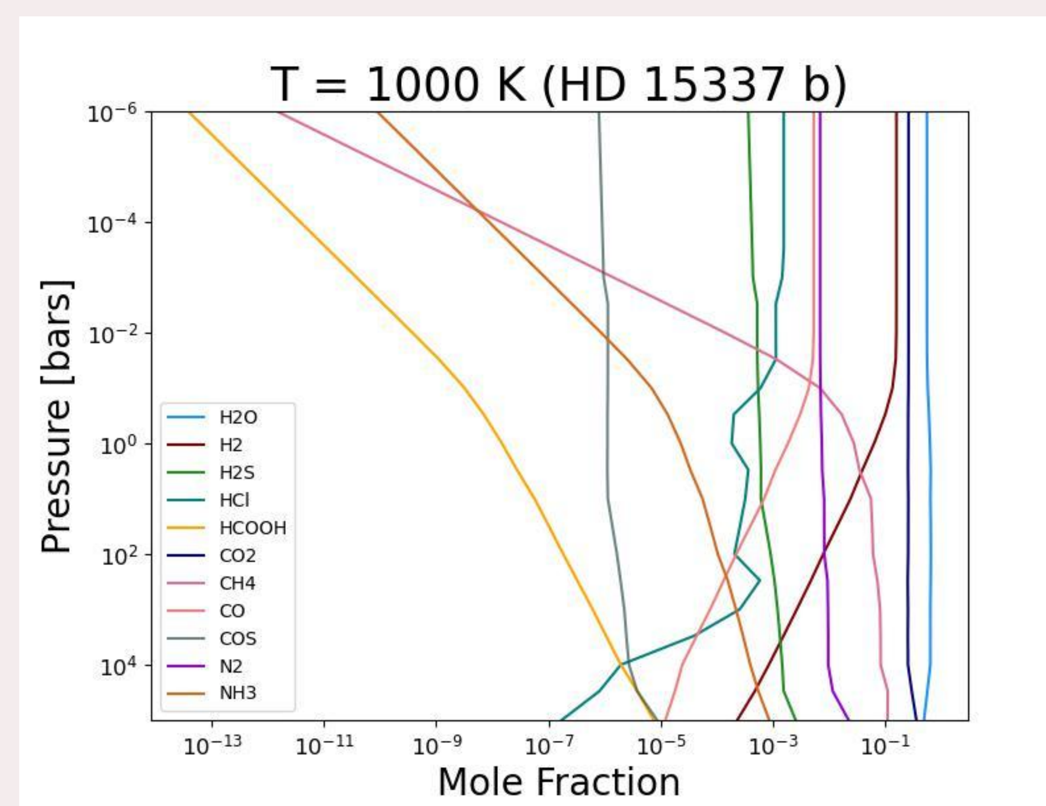
Expected Chemistry of Water Worlds

- To examine the abundances of molecules beyond H_2O and CO_2, we calculated the chemistry for a CI chondrite (bodies with nonvolatile chemical composition closest to that of the Sun) with 16% water by weight at a variety of temperatures and pressures
- We show the chemistry at two temperatures based on observations done by the COMPASS team with JWST in cycles 1 and 2





Chemical abundances for model atmospheres with a temperature of 550 K with 9 species present (above) and 1000 K with 13 species present (below)

- We find a wide range of molecules beyond H_2O and CO_2 present in significant abundance. Clearly, more sophisticated models of water world atmospheres are needed

Next Steps

- **Making edits to PICASO in order to more accurately model water atmospheres**
  - The user will set abundances for any combination of species including CO, H_2O, CH_4, NH_3, CO_2, N_2, HCN, H_2, PH_3, C_2H_2, and Na and PICASO will calculate the opacities on the fly
  - Model H_2O-H_2O collision induced absorption in the atmosphere
  - Use a H_2O/CO_2 mixture as the background gas for calculating gaseous opacities instead of H_2/He
- **Extend the atmosphere down to the surface of the planet**
  - Model interactions between a magma surface and a steam atmosphere as this may change the structure of the lower atmosphere
- **Ultimate goal:**
  - Perform analysis on a water world through all stages
    - Data reduction through COMPASS
    - Atmospheric models using **PICASO**