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Endogenic Water Production and Its Influence on Atmospheric Composition in Sub-Neptunes Using Global Equilibrium Chemistry

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Sub-Neptunes are the most abundant type of exoplanet, yet their formation and evolution remain widely debated. They are often classified into two distinct categories: gas dwarfs, which are water poor and consist primarily of a hydrogen-helium envelope surrounding a rocky core, and water worlds, where a substantial fraction of the planet's mass is composed of water. However, most previous models have primarily considered accretion from the protoplanetary disk as the primary source of water while largely neglecting the role of chemical water production during planetary evolution. A more complete understanding of sub-Neptune formation pathways requires improved modeling of exoplanet interior chemistry, particularly processes that may lead to the endogenous production of water.

A key challenge in addressing this question is the need for a framework that self-consistently models the equilibrium chemistry of a planet's interior and atmosphere. The Schlichting and Young (2022) global equilibrium code (GEC) marks a significant advancement in this regard. It is the first framework capable of determining the equilibrium state of a planet's core, mantle, and envelope, offering detailed insights into the chemical composition of sub-Neptune exoplanets.

Building on this foundation, we significantly improved the original GEC by implementing a gradient descent algorithm, reducing computational time from 1.5 hours to just 10 seconds while simultaneously enhancing numerical accuracy. This breakthrough enables, for the first time, the application of the GEC to large-scale population studies. By incorporating data from the New Generation Planetary Population Synthesis (NGPPS) model, the improved framework facilitates a direct comparison of water content between a traditional accretion model, represented by the NGPPS, and the GEC, which accounts for interior chemistry. The analysis reveals distinct planetary populations, providing strong evidence for endogenic water production. Moreover, results from the GEC indicate that the presence or absence of endogenic water is closely linked to atmospheric composition: planets with substantial endogenic water predominantly have H2-dominated atmospheres (Figure 1), whereas those lacking endogenic water exhibit CH4-dominated atmospheres (Figure 2). These findings underscore the critical role of equilibrium models in advancing our understanding of the chemical evolution of sub-Neptunes and their atmospheres.