PICASO: Modeling Exoplanetary Atmospheres Self-Consistently with Photochemistry and Vertical Mixing

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Abstract

JWST observations of exoplanetary atmospheres have already shown that processes causing disequilibrium chemistry, such as vertical mixing and photochemistry, are extremely important. Apart from being poorly understood, they are already identified as important pathways to probe the interiors and formation pathways of exoplanets. However, to effectively use these processes as probes of deep exoplanetary atmospheres and interiors in the JWST era, they need to be physically understood first, which requires more sophisticated atmospheric models than what is available today. We have developed PICASO 3.0, which is an open-sourced atmospheric model and is coupled with the 1D chemical network code VULCAN, which has allowed us to model the effects of vertical mixing, photochemistry, and molecular diffusion in exoplanetary atmospheres self-consistently. As this model is open-sourced and well-documented, it serves as an important resource for the whole community for modeling *JWST* observations of transiting exoplanets and brown dwarfs.

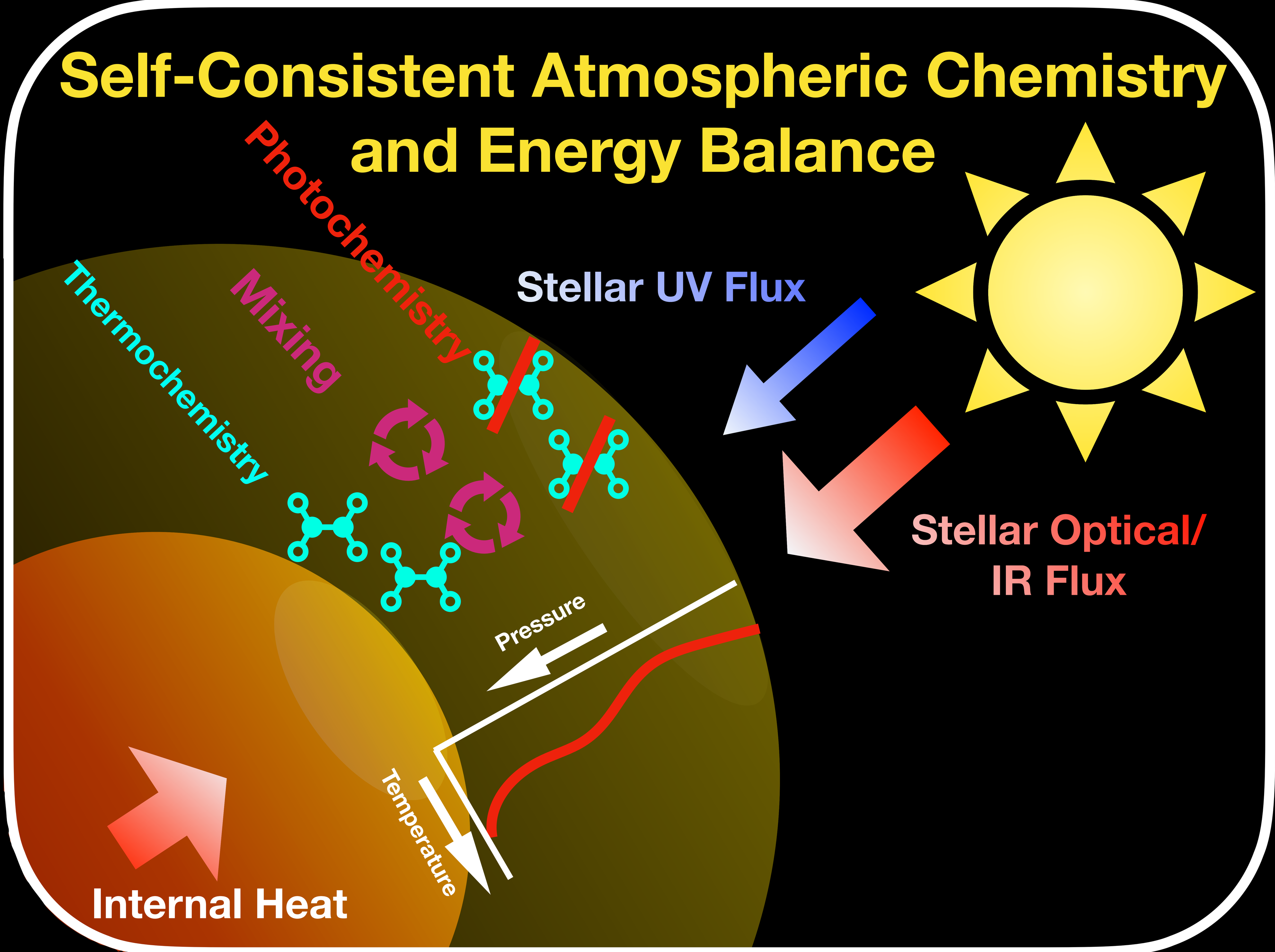
Introduction

Some of the first observations of exoplanetary atmospheres with *JWST* have clearly revealed the presence of photochemical products in the atmospheres of hydrogen-rich gas giant planets (e.g., Rustamkulov et al. (2023), Alderson et al. (2023), Tsai et al. (2023)). The effect of photochemistry on the chemical composition of exoplanetary atmospheres have been explored with 1D chemical kinetics models (e.g., Moses et al. (2011), Tsai et al. (2021)). However, these chemical kinetics models have often assumed that the atmospheric temperature-pressure (*T(P)*) profile is not affected due to vertical mixing of gases or photochemical processes. On the other hand, climate models used to compute atmospheric *T(P)* profiles often ignore the presence of these processes in exoplanet atmospheres and assume thermochemical equilibrium (e.g., Fortney et al. (2008), Goyal et al. (2020)). The schematic shown in the right side shows how each of these assumptions about atmospheric chemistry only works for a specific part of the atmosphere of an irradiated planet. The assumptions of thermochemical equilibrium is perhaps valid for the deeper parts of the atmosphere while the upper atmosphere chemistry is strongly influenced by vertical mixing and photochemistry. Therefore, a more realistic climate model for exoplanetary atmospheres must not rely on assumptions like thermochemical equilibrium throughout the atmosphere.

Why treat disequilibrium chemistry self-consistently?

Atmospheric chemistry and temperature structure are both closely connected together through the wavelength-dependant optical depth structure of the atmosphere. The atmospheric *T(P)* structure influences the detailed chemical composition of the atmosphere which in turn controls the optical depth structure of the atmosphere. The optical depth structure strongly influences the atmospheric radiative transfer which in turn controls the atmospheric *T(P)* profile to maintain energy balance in the atmosphere. Therefore, it is crucial that the chemical compositions of exoplanetary atmospheres and their *T(P)* structure should be calculated simultaneously and self-consistently. Brown dwarf atmospheric models which have treated disequilibrium chemistry self-consistently for their atmospheres have found that it can effect the *T(P)* profile of brown dwarf atmospheres by ~ 100-300 K (e.g., Mukherjee et al. (2022a), Karalidi et al. (2021), Philips et al. (2020)). Therefore, it is crucial that atmospheric chemistry and *T(P)* profiles for exoplanets be evaluated self-consistently and simultaneously.

Self-Consistent Atmospheric Chemistry and Energy Balance



Why treating disequilibrium chemistry self-consistently matters?

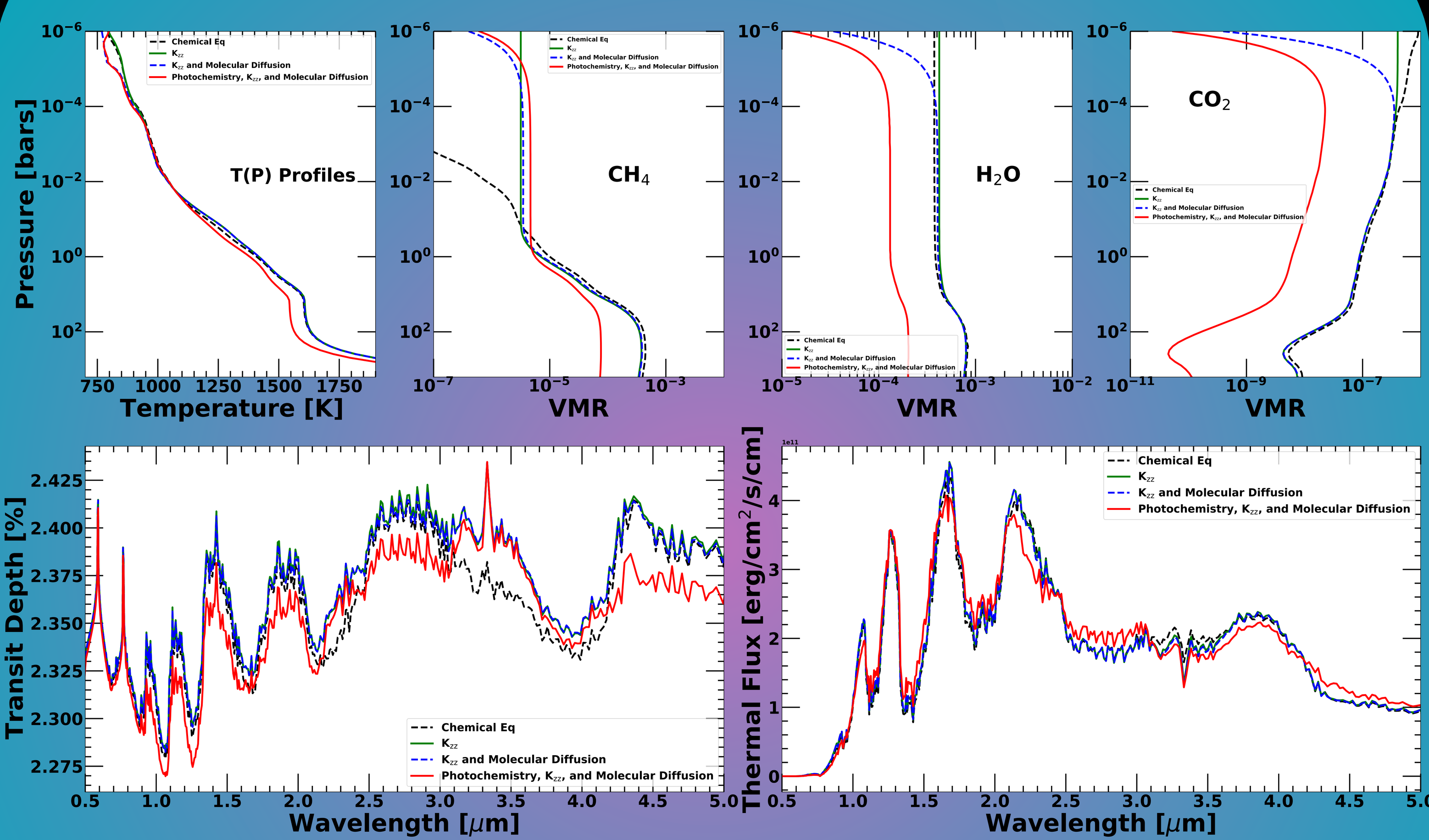


Figure 1 - Effect of various assumptions about atmospheric chemistry on the *T(P)* profile, chemistry, transmission spectrum, and emission spectrum for a solar composition gas giant planet with T_{eq} =1200 K is shown. The top left panel shows the self-consistent *T(P)* profile calculated for the planet assuming chemical equilibrium (black dashed line), chemical disequilibrium due to mixing (solid green line), chemical disequilibrium due to mixing and molecular diffusion (blue dashed line), and chemical disequilibrium due to both photochemistry and mixing (red solid line). The two middle and right panels at the top show the effect of these assumptions on abundances of CH_4, H_2O, and CO_2, respectively. The lower left panel shows the effect of these scenarios on the transmission spectrum of the planet whereas the lower right panel shows the effects for the emission spectra.

Effect of Disequilibrium Chemistry on *T(P)* Profile at different T_{eq}

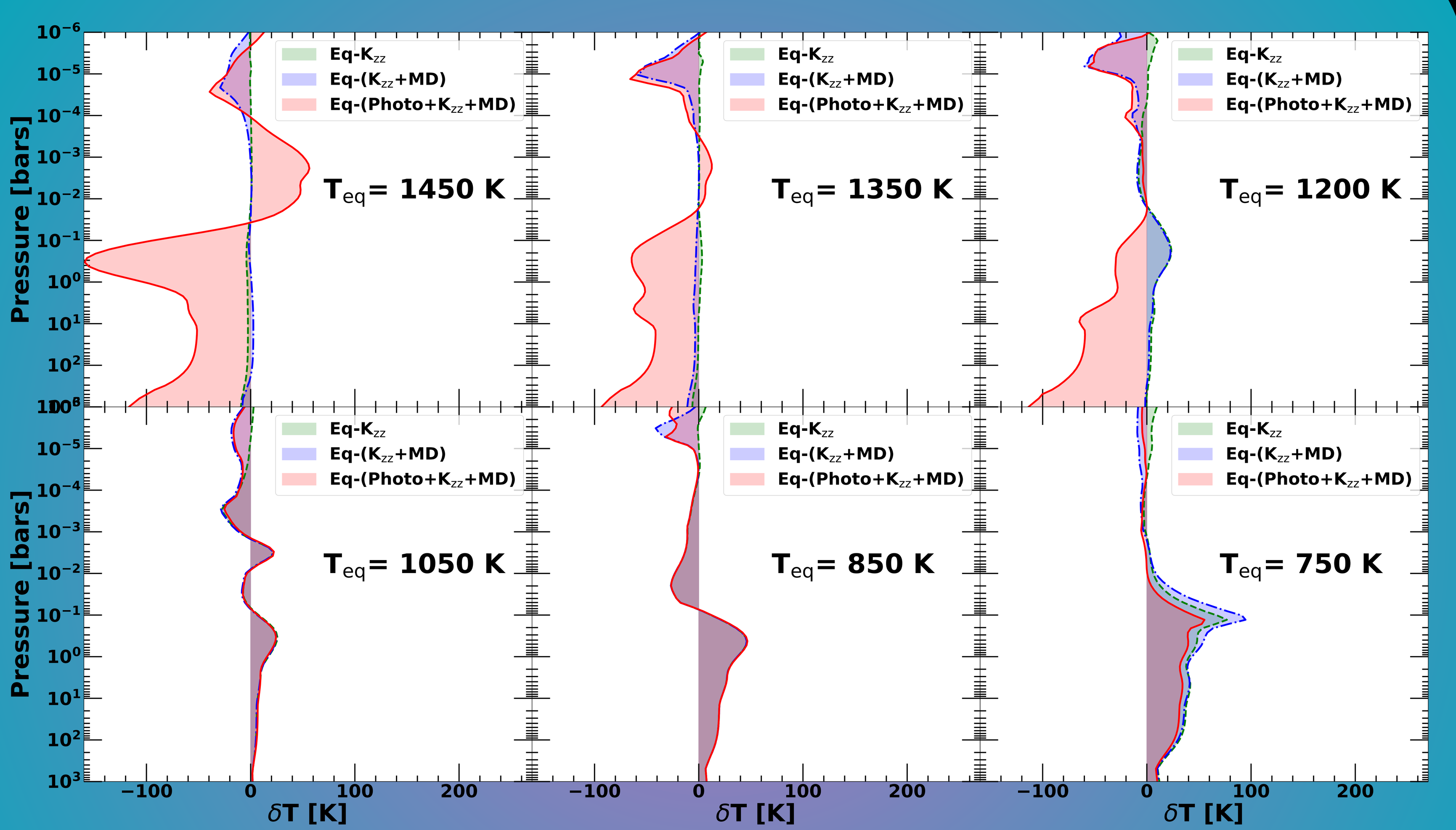


Figure 2 - The difference between the *T(P)* profiles assuming different scenarios of disequilibrium chemistry and the *T(P)* profile calculated assuming chemical equilibrium are shown for various T_{eq} values. Each panel corresponds to a different T_{eq}. The difference between the *T(P)* profiles calculated with photochemistry and chemical equilibrium are shown in red whereas the differences between profiles with just mixing and chemical equilibrium are shown in green. The difference between *T(P)* profiles due to the presence of both mixing and molecular diffusion is shown with blue. For high T_{eq} values (top three panels) photochemistry can lead to ~ 100 K differences in the *T(P)* profile relative to chemical equilibrium while mixing and molecular diffusion can only cause ~20 K differences. For lower T_{eq} atmospheres, all the three scenarios — photochemistry, mixing, and mixing with molecular diffusion cause ~10-50 K differences in the *T(P)* profiles depending on the T_{eq} value.

Results

- We have coupled the publicly available PICASO climate model (Mukherjee et al. (2023), Batalha et al. (2019)) with the chemical kinetics code VULCAN (Tsai et al. (2021)). This has allowed us to calculate self-consistent models of exoplanet atmospheres with photochemistry.
- Figure 1 shows such a model for a hot Jupiter planet with equilibrium temperature T_{eq} = 1200 K. The *T(P)* profile of the same planet was computed self-consistently with four different assumptions about its atmospheric chemistry — chemical equilibrium, presence of mixing, presence of mixing with molecular diffusion, and the presence of photochemistry.
- Figure 1 shows that the model which takes photochemistry into account self-consistently leads to large changes in the atmospheric *T(P)* profile and abundances of gases like CH_4, H_2O, and CO_2 relative to the other three assumptions. This makes it clear that accounting for photochemistry within 1D climate models is crucial instead of post-processing photochemistry over pre-calculated *T(P)* profiles which assume chemical equilibrium.
- In Figure 2, we explore how the impact of photochemistry and vertical mixing on the *T(P)* profile of exoplanets evolves over varying T_{eq}. Figure 2 shows the difference in temperature at each pressure between models with vertical mixing or photochemistry and models assuming chemical equilibrium at various T_{eq}.
- We find that photochemistry can cause changes in the *T(P)* profile by ~ 100 K for highly irradiated planets with T_{eq} > 1200 K while models with just vertical mixing show only ~10 K differences from profiles calculated with chemical equilibrium. Below this T_{eq} value, the impact of vertical mixing on the *T(P)* increases and is ~ 10-50 K depending on the T_{eq} of the planet. The impact of including photochemistry in addition to vertical mixing on the *T(P)* profiles of these warm planet models is rather negligible.
- We also explore how the impact of photochemistry changes depending on the C/O ratio of the planet atmosphere for a hot Jupiter with T_{eq} = 1200 K in Figure 3. We find that photochemistry can cause ~ 200 K changes on the *T(P)* profile and can lead to large changes in the H_2O abundance of very O- rich atmospheres with subsolar C/O. While the impact of photochemistry on the *T(P)* profile of atmospheres with supersolar C/O is negligible, it can still effect its chemistry.

Effect of C/O Ratio

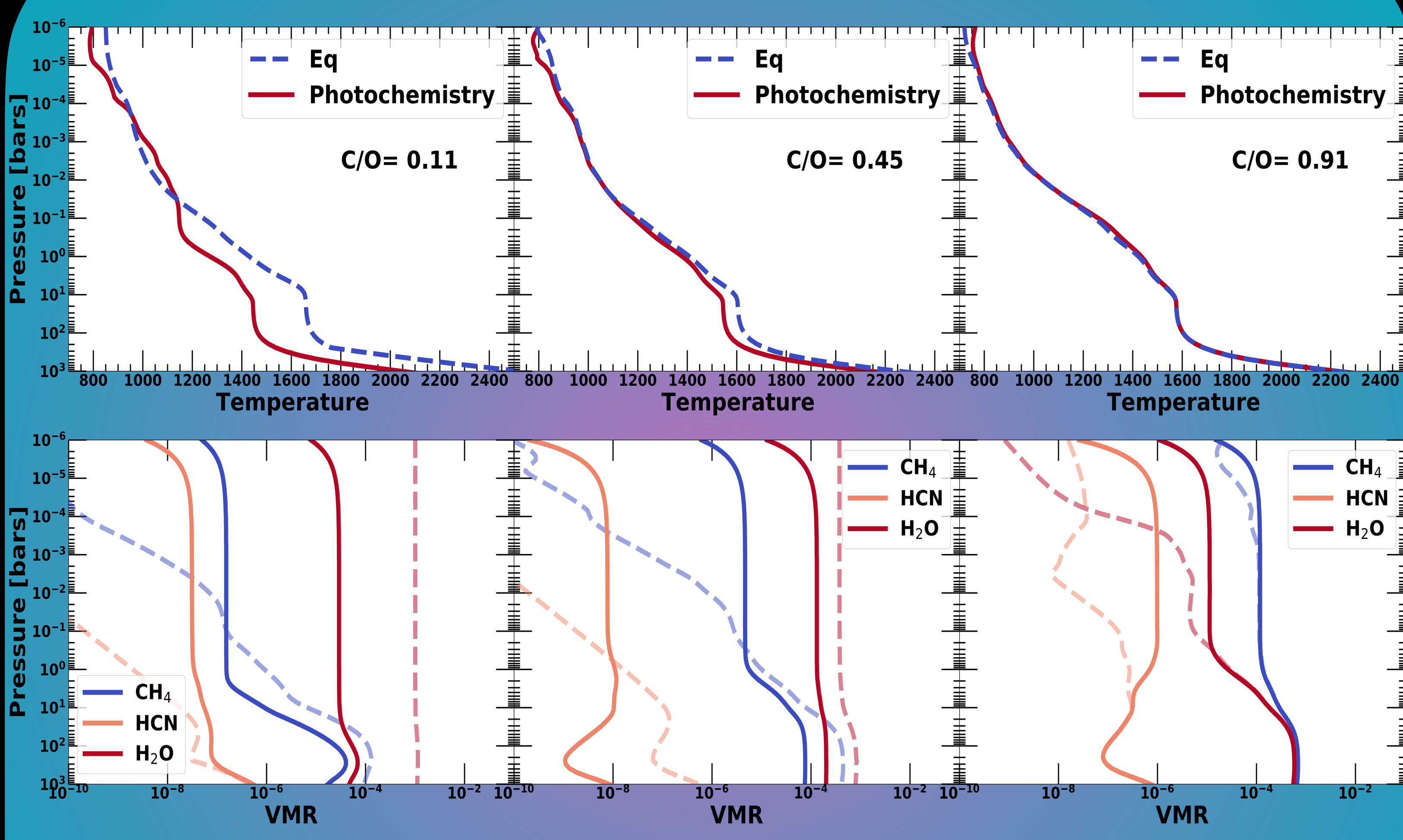


Figure 3- The effect of photochemistry on the *T(P)* profile and atmospheric chemistry at different C/O ratios is shown for a planet with T_{eq} = 1200 K. The top three panels show the comparison of the *T(P)* profile calculated by assuming photochemistry (solid red line) with the profile calculated by assuming chemical equilibrium (dashed blue line) for subsolar, solar, and supersolar C/O ratio in the top left, middle, and right panels, respectively. The bottom left, middle, and right panels show the abundance profiles of CH_4, HCN, and H_2O for the chemical equilibrium scenario (dashed lines) and the photochemical scenario (solid lines) for the three C/O ratios shown in the top panels. The effect of photochemistry on the *T(P)* profiles and atmospheric chemistry is much more pronounced in O- rich atmospheres than in C- rich atmospheres. Photochemistry can cause large changes in the H_2O abundance in very O- rich atmospheres.

Conclusions

- We show that particular assumptions about the chemical processes in the atmospheres such as photochemistry or vertical mixing can cause large changes to the *T(P)* profile of the atmosphere of gas giant exoplanets relative to the *T(P)* profiles computed by assuming thermochemical equilibrium.
- For a solar composition of a gas giant exoplanet, we quantify the effect of chemical processes such as photochemistry or vertical mixing on the *T(P)* profile of the atmosphere as a function of the planet's T_{eq}. We find that for planet's with T_{eq} > 1200 K, photochemistry can cool down the atmospheric *T(P)* profile by ~ 100 K relative to the *T(P)* profile computed by assuming chemical equilibrium.
- For planets with T_{eq} higher than 1200 K, the effects of vertical mixing alone on the *T(P)* profile is rather negligible but its impact on the *T(P)* profile of colder planets is higher and of the order of ~10-50 K. For these warm Jupiters, the impact of photochemistry on their *T(P)* profiles are rather negligible.
- We also explore how the impact of photochemistry on the atmospheric *T(P)* profile changes with different C/O ratios. We find that for O- rich atmospheres (subsolar C/O) the effects of photochemistry on atmospheric *T(P)* profile and chemical abundances is huge while for C- rich atmospheres (supersolar C/O) its impact on the *T(P)* profile is negligible but it still causes changes to atmospheric chemistry.
- In future, we aim to explore how other variations in very important atmospheric parameters like the intrinsic temperature, vertical mixing parameter K_{zz}, and atmospheric metallicity cause changes to the atmospheric *T(P)* profile and chemistry in the presence of photochemistry.

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