Reduction of photochemical networks : application to sulfur chemistry for 3D atmospheric models

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Abstract

The detection of SO_2 in four different exoplanet atmospheres (WASP-39 b, WASP-107 b, HAT-P-26 b, GJ 3470 b) by the James Webb Space Telescope (Tsai et al., 2023; Dyrek et al., 2024; Beatty et al., 2024; Gressier et al., 2025) has proven the importance of sulfur chemistry in current models to better understand exoplanets and prepare future missions like ARIEL. More specifically, photochemistry has been identified as the key process responsible for oxidizing H_2S to SO_2, and is essential to explain the abundances inferred from these observations. Such processes are currently modeled in the literature using detailed chemical networks in one-dimensional models, but other applications such as in retrievals or GCMs require a fast, reduced network.

In this talk, we will discuss the reduction of detailed chemical networks for exoplanet atmospheres subject to photochemistry. We'll use results from graph theory to discuss the different approaches that can be used to construct a graph from this chemical network, analyze the chemical pathways and identify key reactions and intermediates that connect the targeted species. We'll discuss how this methodology can be applied to construct a reduced chemical network from 1D simulations with FRECKLL (Al-Refaie et al., 2024), and compare it to more black box approaches that have been used previously in the literature such as Genetic Algorithms (Lira-Barria et al., 2024). We'll use both of these approaches to reduce a detailed C/H/O/N/S kinetic network that has been built and validated on experimental data in a previous work (Veillet et al., 2026), apply it to the case study of sulfur chemistry on WASP-39 b and WASP-107 b, and discuss the utility of these tools for chemical analysis, 3D modeling and on-the-fly reduction in retrievals.

References

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