EPSRC DTP Summer Internships 2024
Going beyond JWST with combustion chemistry

Background

Photochemistry is a fundamental process of planetary atmospheres that regulates the atmospheric composition and stability. However, the detection of photochemical products in exoplanet atmospheres has remained elusive until very recently. First observations from the JWST Transiting Exoplanet Community Early Release Science Program have found a spectral absorption feature at 4.05 µm arising from sulfur dioxide SO_2 in the atmosphere of WASP-39b. A suite of 1D photochemical models have recently showed consistently that the most plausible way of generating this SO_2 spectral feature at 4.05 µm was through photochemical processes (Tsai et al., 2023; Fig. 1).

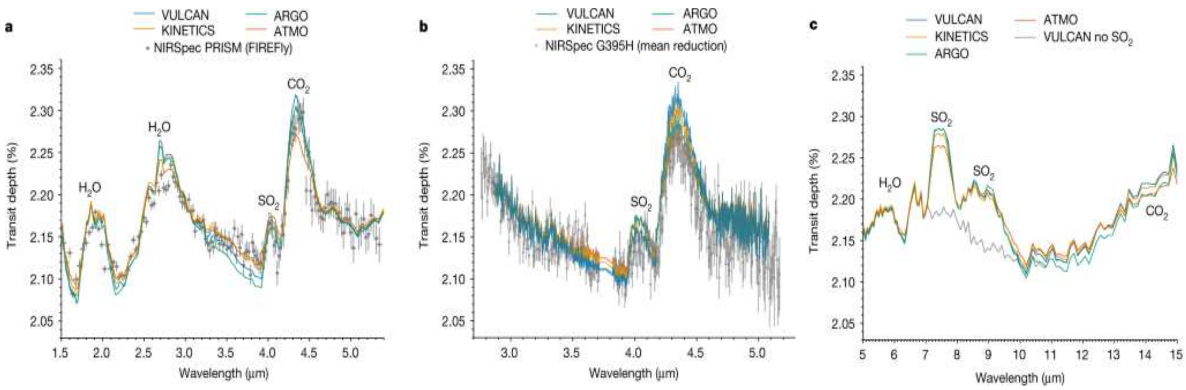

Fig. 1 (adapted from Tsai et al.. 2023): Transmission spectra averaged over the morning and evening terminators generated from 1D photochemical model results. a, Comparison with the NIRSpec PRISM FIREFly reduction. b, Comparison with the NIRSpec G395H weighted-mean reductio9. c, Predicted spectra across the MIRI LRS wavelength range, with SO_2 removed from the VULCAN output shown in grey to indicate its contribution. All of the spectral data show 1σ error bars and the standard deviations averaged (unweighted) over all reductions are shown for the NIRSpec G395H data.

As a part of this suite of 1D photochemical models which have been successfully applied to the atmosphere of WASP-39b to explain and predict the observations of SO_2 spectral features by JWST is ATMO, a flexible 1D/2D photochemical model developed at the University of Exeter. ATMO includes a complete treatment of radiative transfer as well as a sophisticated photochemical network and has already been applied successfully to the planetary atmospheres over a wide range of temperatures, from brown dwarfs to hot Jupiters (Drummond et al., 2016; Phillips et al., 2020).

Aims & Methodology

These first results from JWST, no matter how far-reaching, are still limited. First, the chemical scheme used by this suite of 1D photochemical models is limited and has not been properly validated. Secondly, the restricted dimensionality of these models, including 1D ATMO, is not able to capture the multidimensional, 2D or even 3D, nature of an exoplanet atmosphere (e.g., Zamyatina et al., 2024). It is time to investigate further - and with more confidence - the observability and spatial variability of various spectral signatures, including those of SO_2, and assess whether they could be detectable with both current and future spectroscopic instruments, including JWST and Ariel.

In this project, we will:

(1) implement into ATMO a brand-new chemical scheme relying on a more comprehensive, robust, and reliable network, extensively validated against combustion experiments over a large range of pressures (0.01-500 bars) and temperatures (300-2500 K). (Veillet et al., 2024; Veillet et al., in prep),

(2) compare your new results to the initial JWST observations and modelled results, and extend the original study even further by exploring the 2D variability of various chemicals and their spectral signatures, including SO_2, using a 2D version of ATMO that has been recently developed and tested through a proven methodology (Roth et al., 2021).

Outcomes and Products

Once ATMO has been adapted, we will use the updated code to answer three questions:

1) What further constrains (e.g., metallicity, C/O ratios) can we derive from the comparison of JWST observations with numerical simulations relying on extensively validated and recent state-of-the-art combustion networks?

2) Can we predict some sort of spatial variability (e.g., limb asymmetry) for various spectral signatures, including those of SO_2 using models able to capture the multidimensional nature of exoplanetary atmospheres?

3) Would that spectral variability be detectable with both current and future spectroscopic instruments, including JWST and Ariel?

References

Drummond et al. "The effects of consistent chemical kinetics calculations on the pressure-temperature profiles and emission spectra of hot Jupiters". *Astronomy and Astrophysics* 594, A69, DOI: 10.1051/0004-6361/201628799.

Phillips et al. "A new set of atmosphere and evolution models for cool T–Y brown dwarfs and giant exoplanets" *Astronomy and Astrophysics* 594, A69, DOI: 10.1051/0004-6361/201937381.

Roth et al., "Pseudo-2D modelling of heat redistribution through H_2 thermal dissociation/recombination: consequences for ultra-hot Jupiters" *Monthly Notices of the Royal Astronomical Society* 505, 4515–4530 (2021) DOI: 10.1093/mnras/stab1256

Tsai et al., "Photochemically produced SO2 in the atmosphere of WASP-39b", *Nature* 627, 483-487 (2023). DOI: 10.1038/s41586-023-05902-2.

Veillet et al., "An extensively validated C/H/O/N chemical network for hot exoplanet disequilibrium chemistry" *Astronomy and Astrophysics* 682, A52 (2024). DOI: 10.1051/0004-6361/202346680.

Zamyatina et al., "Quenching-driven equatorial depletion and limb asymmetries in hot Jupiter atmospheres: WASP-96b example" *Monthly Notices of the Royal Astronomical Society* 529, 1776–1801 (2024) DOI: 10.1093/mnras/stae600

Noticing the overlap of conditions between the atmospheres of warm/hot exoplanets and car engines (same elemental composition, same P-T range), Dr. Éric Hébrard has been contributed for the past decade to the release of comprehensive chemical networks which **successful bridge combustion chemistry and astrophysics** (e.g, Veillet et al., 2024). He has also been responsible for a new, original and flexible strategy for evaluating both the accuracy and precision of complex chemical models and identifying key chemical formation pathways in combustion chemistry (Hébrard et al., 2015). Dr. Éric Hébrard has also been directly involved in experimental measurements of VUV absorption cross-sections through several campaigns that have been performed in synchrotron facilities, which resulted in the study of the thermal variation of absorption cross-section for various chemicals of interest for exoplanetary atmospheres (Venot et al., 2018).

Thanks to a close collaboration with combustion experts, Dr. Éric Hébrard's network of international collaborators is the only team in the world capable of providing highly reliable astrochemical data validated against experimental data.