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Towards a more complex description of chemical profiles in exoplanets retrievals: A 2-layer parameterisation

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Abstract

State of the art spectral retrieval models of exoplanet atmospheres assume chemical profiles which are constant with altitude/pressure. This assumption is justified by the information content of currently available datasets which do not allow, in most cases, for the molecular/atomic abundances as a function of atmospheric pressure/altitude to be constrained. In the context of the next generation of space telescopes, a more accurate description of chemical profiles with additional levels of flexibility may become crucial to interpret observations and gain new insights into atmospheric physics. We explore here the possibility of retrieving pressure-dependent chemical profiles from transit spectra as recorded by future space observatories, without injecting any priors from theoretical chemical models in the retrieval algorithms. The "2-layer" retrieval parameterisation presented here allows for the independent extraction of molecular/atomic abundances above and below a certain atmospheric pressure. By simulating various cases, we demonstrate that this evolution from the assumption of constant chemical abundances is justified by the information content of transit spectra provided by future space instruments. Comparisons with traditional retrieval models show that assumptions made on chemical profiles may significantly impact retrieved parameters, such as the atmospheric temperature, and justify the attention we give here to this issue. We find that the 2-layer retrieval is able to accurately capture discontinuities in the vertical chemical profiles, which could be caused by disequilibrium processes – such as vertical mixing or photo-chemistry – or the presence of clouds/hazes. The 2-layer retrieval could also help to constrain the composition of clouds and hazes by exploring the correlation between the chemical changes in the gaseous phase and the pressure at which the condensed/solid phase occurs. The 2-layer retrieval presented here therefore represents an important step forward in our ability to constrain theoretical chemical models and cloud/haze composition from the analysis of future observations.

1. Introduction

This paper explores the importance of moving towards a more complete description of chemical profiles through the analysis of simulated transit data from JWST [1], Ariel [2] and other future telescopes. In that context, we consider the example of a 2-layer parametrisation with 3 degrees of freedom and the possibility to retrieve these profiles on simulated data using the TauREx retrieval suite [3].

2. Main ideas

Below, Figure 1 shows the comparison of the 2-layer retrieval with the 1-layer constant chemistry model. While both models seem to fit correctly the input 2-layer spectrum, the constant retrieval is not able to recover the appropriate temperature (2100K instead of 1500K). The 1-layer model compensate the lack of flexibility in the chemical profiles by increasing the temperature. This sort of degeneracy could lead to wrong physical interpretation of exoplanet atmospheric observations. However, provided that both models are tested, the nested sampling evidence shows a clear preference for the 2-layer retrieval.

The 2-layer model has also been tested on simulated cases of an ultra-hot Jupiter (similar to Wasp 33b) and a sub Neptune type planet (similar to GJ 1214b [4]). These cases highlighted the additional level of information provided by the 2-layer retrieval as it allowed to access new physical phenomena:

- Detection of chemical layers such as TiO present only in the top atmosphere.

- Characterisation of hydrocarbon clouds by correlating the apparition of condensates at a given altitude with de reduction of CH_4 abundance by photochemistry.

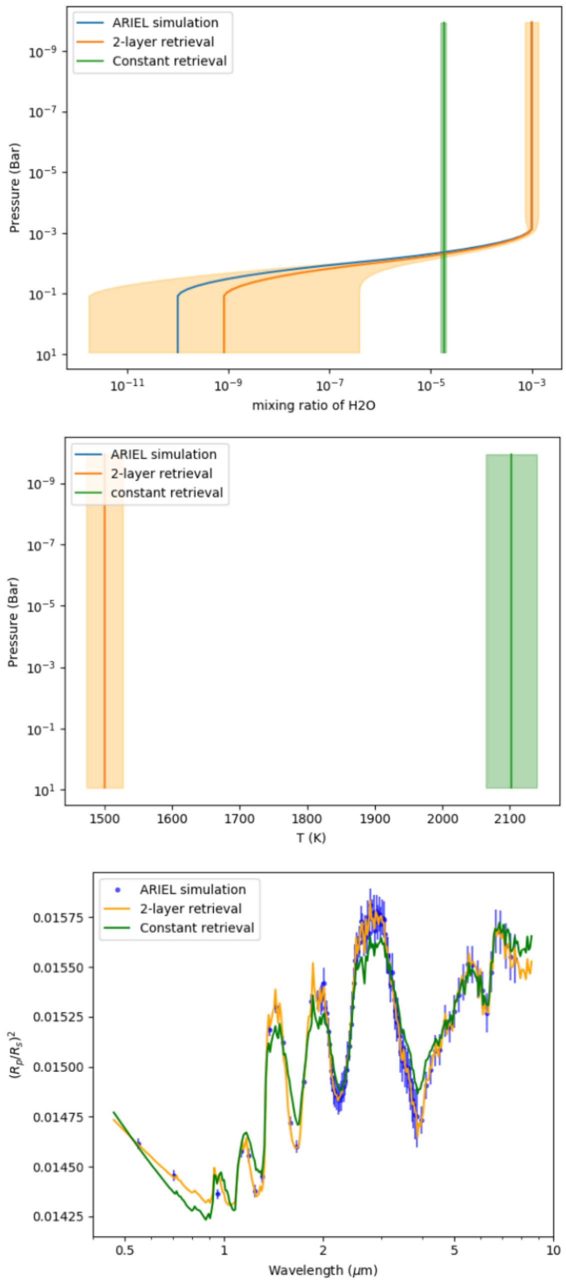

Figure 1: Retrieved chemical profiles (top), temperature profiles (middle) and best fit spectra (bottom) of a 2-layer model (orange), a 1-layer model (green) on a 2-layer simulated observation (blue).

3. Summary and Conclusions

In this paper we have assessed the possibility of constraining the abundance as a function of altitude of key chemical species present in exoplanet atmospheres. We have used simulated JWST and Ariel transit spectra to test whether the data quality of the next generation of space-based instruments will allow for the retrieval of vertical chemical profiles. We found that the 2-layer retrieval is able to capture accurately discontinuities in the vertical chemical profiles, which could be caused by disequilibrium processes – such as vertical mixing or photo-chemistry – or the presence of clouds/hazes.

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