SF2A 2024
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THE MAGIC TRIPTYCH TO CHARACTERISE THE ATMOSPHERES OF EXOPLANETS: OBSERVATIONS, MODELLING, EXPERIMENTS

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Abstract. In this introductory talk of the workshop 'Characterizing planetary atmospheres through experiment, modelling and observation', I have focused on the study of exoplanets. The aim is to show how complementary are these three approaches to improve our knowledge of these worlds, and give an overview (not exhaustive !) of some recent works and developments conducted in each of them.

Keywords: exoplanets, atmospheres, experiments, modelling, observation

1 Introduction

Since the discovery of the first exoplanet, thirty years ago, more than 5600 have been confirmed up to June 2024*. These detections reveal the large diversity of worlds that exist in the Universe, and the unique character of our Solar System. One of the main current motivations of our scientific community regarding these planets is to understand how they formed and evolved. To answer these questions, the key is to observe their atmosphere in order to determine their chemical composition and in particular to retrieve the elemental abundances (e.g. Kama et al. 2019; Turrini et al. 2021; Pacetti et al. 2022). Infrared transmission spectroscopy is the main method to have this information, as the molecules present in the planetary atmospheres absorbs the stellar light and thus imprint their signature on the measured spectra. This is the method used by the past, current, and future, space telescopes Hubble, Spitzer, James Webb or Ariel.

These kind of observations are performed since about 15 years on warm giant exoplanets. The first observations reveal (or suggest) the presence of molecules, such as water (H_2O), methane (CH_4) and carbon dioxide (CO_2), in the atmosphere HD189733b (Swain et al. 2009b) and HD209458b (Swain et al. 2009a).

However, to go from raw observational data to these detections, models as well as experiments are mandatory. I will present in the Sect. 2 the different types of models existing and in Sect. 3 how experiments are necessary to feed and improve models.

2 Link between models and observations

My goal here is not to go into detail about the different existing models, nor to give an exhaustive list. I only want to highlight that the use of models is essential at each stage of data processing and analysis. Basically, there are three main stages to go from raw data to the interpretation (noting that the distinction between stages 2 and 3 is not strict and can be coupled):

- First step: data reduction & calibration with pipelines. This step can be performed with codes such as Iraclis, Cascade, tshirt, Eureka !, Tiberius, FIREFLY, TEATRO, SPARTA ...

- Second step: data analysis with Radiative Transfer Models (e.g. ScCHIMERA, PICASO, PHOENIX, ATMO, ExoREM, Lavvas et al., ...) or Retrieval Models (e.g. TauREx, NEMESIS, CHIMERA, PYRAT BAY, petitRADTRANS, Brogi & Line)

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- Third step: interpretation with atmospheric models. Here, a large diversity of models exists depending on their main focus. For instance, some codes focus on clouds microphysics (CARMA), on chemical kinetics (e.g. KINETICS, Venot et al., FRECKLL, VULCAN, ATMO, Lavvas et al.), or on the global atmospheric circulation, the so-called GCM (e.g. SPARC/MITgcm, LMD-Z / PCM, UM)

To interpret correctly the observations, these models had to develop and increase their complexity. For instance, the number of dimensions, the inclusion of aerosols, clouds, or disequilibrium chemistry ...

2.1 Evolution of retrieval models

For instance, for retrieval models, the classic assumption is to consider a one-dimensional model and atmospheric abundance profiles constant with altitude. This assumption is called 'free' chemistry (Waldmann et al. 2015). However, atmospheric kinetic models, taking into account the disequilibrium processes (i.e. mixing and photodissociations), show that such behaviour might be correct for some molecules, but not for all of them (see for instance the composition of WASP-43b in Venot et al. 2020b, or WASP-39b in Tsai et al. 2023). Variations of the abundances are expected due to the change of temperature with pressure/altitude, as well as effect of disequilibrium processes (i.e. quenching, photochemistry). Several developments have been undertaken in recent years to better take into account this variability with altitude:
- Changeat et al. (2019) implemented in the TauRex retrieval code a 2-layer parameterization which makes it possible to properly capture the discontinuities of the vertical chemistry profiles.
- Then, the next step was to include the thermochemical equilibrium calculation in TauRex, in order to make retrievals compatible with the composition at thermochemical equilibrium. Three codes (ACE, FastChem and GGChem) have been coupled thanks to the plugins system of TauREx 3.1 (Al-Refaie et al. 2022). The advantage of having several codes available is that they do not all include the same species and the same processes (condensation is not included in ACE for example). Retrievals using thermochemical equilibrium are generally better than those using the classical 'free' hypothesis, however, Jaziri et al. (2024) shows that depending on the planets, this is not always true, because of the too strong constraint on the chemistry brought by these codes. In some cases, the 'free' hypothesis, giving more freedom, can be better.
- Finally, the last development implemented in the retrieval code TauREx is to consider disequilibrium composition. This has been possible thanks to a coupling with the kinetic 1D code FRECKLL (Al-Refaie et al. 2024). The tests carried out on synthetic data show that the fits are much better with this new model than with the hypothesis of thermochemical equilibrium, however such a retrieval also brings many constraints and induces a bias due to the chosen chemical network. For example, if we consider a complete chemical scheme, or reduced/simplified without photodissociation, it will still be possible to obtain a good fit of the spectrum, but the retrieval of the abundance profiles will not be correct. However, the result obtained is still better than the retrieval assuming thermochemical equilibrium. In conclusion, coupling a retrieval model to a kinetic model is a huge progress, but it is a solution that also has its limitations, since it will integrate the problems of kinetic models. This aspect will be developed in the next Section.

3 Link between experiments and models

All atmospheric models, whatever the physical or chemical processes they are focused on, need to use physicochemical data, that might be calculated theoretically, determined experimentally, or a combination of both approaches. Laboratory astrophysics is thus crucial to feed models. In this Section, I will give some examples of works carried out with this in mind.

3.1 Chemical schemes

One of the main ingredients of kinetic models is the chemical scheme used, that is to say the list of species, reactions, and the associated rate coefficients. It has already been shown that different chemical schemes lead to different results on the chemical composition, because different levels of quenching (Venot et al. 2012; Moses 2014). These differences can then generate different interpretations of the observations. It is therefore fundamental to have a reliable chemical scheme adapted to the temperatures encountered in exoplanets, in particular, to take into account the endothermic reactions, happening at high temperature. Thus, the question is: how can we generate reliable chemical schemes? How can we be sure that our models give correct predictions? Unlike planets of our Solar System, it is not possible to send probes in the atmospheres of exoplanets in

order to make in-situ measurements, and the IR spectroscopic observations do not provide sufficiently precise information to constrain our models. Rather, the models are used to interpret the observations. The solution is therefore to carry out laboratory experiments to constrain, improve or validate these models. This is for instance what is done since several years to develop chemical schemes, thanks to an interdisciplinary collaboration between Laboratoire Réaction et Génie des Procédés (LRGP) and Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA). Indeed, chemistry occurring at high temperatures has been studied for many years in this field, particularly for industrial purposes. Many experiments have been conducted in different conditions, with different types of reactors and we can thus use these data sets to build chemical schemes for exoplanetology studies. These chemical schemes validated against experimental combustion data are very robust (Venot et al. 2012, 2015, 2020a; Veillet et al. 2024).

3.2 Atmospheric Chamber Simulation

Another axis of experimental studies consists in recreating an atmosphere in the laboratory and performed different kind of measurements. For instance, it is possible to study the change in chemical composition, particularly under the action of irradiation, but also to measure physico-chemical properties.

3.2.1 Aerosols

In an experiment developed at the Jet Propulsion Laboratory (JPL) by Fleury et al. (2020), it is possible to reproduce and study the formation of aerosols in the atmospheres of hot exoplanets. Then, the high-temperature properties (particularly optical indices) that are very little known, can be determined. Such data is very important for interpreting spectra that present aerosol signatures.

3.2.2 Photochemistry in laboratory

With this same device, it is also possible to reproduce photochemical processes. Fleury et al. (2023a) study in particular the production of hydrocarbons as a function of temperature. Comparing experimental measurements with simulation results makes it possible to identify the processes responsible, or in the event of disagreement, point out key processes that may be missing in models, or eventually key reactions whose reaction rates must be re-evaluated. This combination of experimental and modelling approaches is key to improving our understanding of chemical processes and therefore of exoplanet atmospheres.

3.2.3 Absorption cross-sections

With other experimental devices, such as the UV platform developed at LISA (Poveda 2023), it is possible to measure physico-chemical data that are used by atmospheric models, such as UV absorption cross sections. These data are essential for calculating the photodissociation rates of molecules and radiative transfer, but their thermal dependence is very poorly known, which generates a high uncertainty in the model results and therefore in the interpretation of observations. It has been shown for CO_2 that the absorption increases by several orders of magnitude together with temperature and that this new data has an important impact on the atmospheric composition (Venot et al. 2013, 2018). Recently, the absorption cross-section of C_2H_2 has also been studied (Fleury et al. 2023b, 2024)

4 Conclusions

There are many other models, development of models (going from one to two, then three dimensions to take into account the real geometry of exoplanets) that I don't mention in this proceeding. There are other experiments, other data that can be measured in the laboratory. The goal here is not to do a complete review, which would have been impossible in a talk of fifteen minutes (or in this proceeding), but the objective is above all to show the complementarity that exists between these different axes and to show that combining these different approaches is essential if we want to study the atmospheres of exoplanets. That is why I call it the magic triptych!

O.V. thanks the organisers of the workshop 'Characterizing planetary atmospheres through experiment, modelling and observation' for the invitation to give this introductory review talk, as well as the Conseil de la SF2A for the organisation of this week. O.V. acknowledges funding from the ANR project 'EXACT' (ANR-21-CE49- 0008-01) and from the Centre National d'Études Spatiales (CNES).

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