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Characterization and modelling of exoplanetary atmospheres

Caractérisation et modélisation des atmosphères exoplanétaires

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Abstract. The spectral characterization of exoplanetary atmospheres is a relatively new subject. Until recently, space and ground-based observatories allowed only a few planets to be observed with spectroscopic instruments. The arrival of JWST data and the development of new instruments on Earth will drastically modify the situation, giving access to deeper modelling contraints and to a better understanding on planet formation and evolution. This paper is devoted to describe the turning point experienced by the astronomy of exoplanets that will continue in particular with the launch of the ESA/Ariel mission at the end of the decade.

Résumé. Cet article passe en revue les récentes avancées en physique des atmosphères des exoplanètes, dans le cadre de la préparation de la mission Ariel de l'ESA. La modélisation des atmosphères, bâtie sur les modèles planétologiques développés dans l'étude du Système Solaire, peut aujourd'hui être extrapolée aux exoplanètes par l'utilisation de bases de données moléculaires adaptées aux températures rencontrées. L'une des difficultés des modèles repose sur la forte dégénérescence dans l'inversion des paramètres de structure et composition atmosphérique. Les méthodes bayesiennes d'inversion ont permis des avancées récentes, sur les observations à basse résolution du Hubble Space Telescope, et sont préparées pour les prochaines observations du James Webb Space Telescope. Les avancées attendues dans les prochaines années dans le domaine font de la caractérisation par spectroscopie des exoplanètes une des branches les plus actives du domaine.

Keywords. Exoplanets, Atmospheres, Models, Retrieval, James Webb space telescope (JWST), Ariel mission.

Mots-clés. Exoplanètes, Atmosphères, Modèles, Inversion, Téléscope spatial James Webb (JWST), Mission Ariel.

Note. Follows up on a conference-debate of the French Academy of Sciences entitled "Exoplanets: the new challenges" held on 18 May 2021, visible via https://www.academie-sciences.fr/fr/Colloques-conferences-et-debats/exoplanetes.html.

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1. Introduction

After 25 years devoted mostly to the detection and statistical sampling of general parameters of exoplanets, the spectral characterization enters in a mature stage, with both modelling improvements and new observations. This article will describe some of the recent developments in the field, which are important for the preparation of the Ariel ESA mission currently in development phase. The JWST observations which are just at their beginning will certainly increase our knowledge in a near future and this article will also raise the most important questions to be addressed with both ground-based and space mission of the decade.

2. Observations of exoplanetary atmospheres

2.1. *Observations of the solar system—historical achievements*

The observations of the planets of the solar system are naturally a first basis on which the models of exoplanets are built. Scientists are nevertheless immediately confronted with the question of the specificity of the Solar System. The anthropocentrism encountered in the history of astronomy must be avoided before extrapolating our knowledge of planets to exoplanets. Among examples of unsafe extrapolations are the search for life on Mars, with announcement of vegetation detection in the 1950's [1]. However, the physical mechanisms can be studied with unparalleled precision on nearby objects and then applied to different systems: this is the case in the major fields of radiative transfer, meteorology, Earth–Sun interactions, etc. The utility of the Solar System observations is therefore important to describe detailed physical mechanisms, before extrapolation is made to other planets. The interpretation of planetary atmospheres of Solar System objects has been developed since the space era and the first planetary missions of the 1960s–1970s. The questions were approached from terrestrial models (atmospheric structure, meteorology, radiative transfer, aeronomy), by pointing out the Earth–Planet relations in the physics of the atmospheres. It is the same paradigm that we live today by passing from planets to exoplanets. The planets, thanks to the close observations, even in situ, allow us to validate the physical models which will have to be extrapolated to different conditions in the exoplanets.

2.2. *Past and future observations of exoplanetary atmospheres: which constraints for atmospheric models?*

Observations of exoplanetary atmospheres come almost exclusively from transiting and directly imaged exoplanets. For transiting exoplanets, the atmosphere can be probed: (1) during transit by measuring the variation of planetary radius caused by molecular/atomic absorption with wavelength (technique called transit spectroscopy), (2) during the eclipse by measuring the thermal emission or reflected light from the exoplanet (technique called eclipse spectroscopy), (3) during the whole orbit by measuring the variation of thermal emission or reflected light (technique called phase curve observation). The first observation of an exoplanetary atmosphere was obtained by transit spectroscopy of sodium lines in the atmosphere of HD209458 b, although this detection is still debated [2–5]. Most of JWST exoplanet observations will be dedicated to transit/eclipse spectroscopy and phase curves. For directly imaged exoplanets, one can measure the thermal emission spectrum of the planet and detect molecular absorption. Future telescopes, like the Roman Space Telescopes or the ELTs will detect reflected light of temperate exoplanets. The characterization of exoplanetary atmospheres by these different techniques is now done routinely. New data of exoplanetary atmospheres are published every week. After 20 years, a large list of molecules/atoms detected in exoplanetary atmosphere has now been established (H_2O, CO, CH_4, NH_3, CO_2, HCN, C_2H_2, H, He, Na, K, Li, Mg, Ca, Fe, V, Cr,...) [6, 7]. A surprise was to discover that most exoplanets are cloudy or hazy [8]. The presence of these aerosols is currently one of the main limitations in our ability to probe the chemical composition of exoplanetary atmospheres. Another major breakthrough on exoplanetary climates came from the detection of equatorial superrotation on hot Jupiters from thermal phase curves [9]. The fast equatorial jet redistributes heat to the nightside and produces an eastward shift of the hot spot on strongly irradiated exoplanets. Superrotation was predicted by atmospheric modelers a few years before its detection [10]. Exquisite measurements of phase curves will be obtained in the coming years with JWST revealing the horizontal variations of temperature, chemical composition and clouds. These would be strong constraints for atmospheric models able to couple atmospheric dynamics, thermal structure, chemistry and clouds.

One of the main goals is now to measure molecular abundances in order to provide constraints on exoplanet formation mechanisms. A major question for the coming decade is to determine the nature of sub-Neptunes, planets with radii between 1.8 et 3 Earth radii, which are very abundant in our galaxy but with no equivalent in our solar system. These planets could be composed of a rocky core surrounded by a H_2-dominated atmosphere or they could be water-worlds with a H_2O-dominated atmosphere. The last case would imply formation of these planets beyond the ice line and migration toward their host stars. Another big question concerns the evolution of the atmospheric metallicity (the fraction elements higher than H and He) as a function of the planetary mass. Giant planets in the solar system show a decrease of the atmospheric metallicity with the planetary mass following a simple scaling law. A generalization of this trend to exoplanets would be a major constraint for planetary formation models. However, measurements of atmospheric metallicity based on water vapor abundance in exoplanet atmospheres do not show such a correlation with often a low metallicity, sometimes even lower than solar [6]. Better measurements will be required to break the degeneracies caused by the presence of clouds/hazes but there seems to be a large diversity in exoplanetary atmospheres. Another motivation for the chemical characterisation of exoplanetary atmosphere is the possible link between the atmospheric C/O ratio and the planetary formation mechanism. Models predict variations of this ratio in the gas and solids of protoplanetary disks depending on the location of the different ice lines (H_2O, CO_2, CO) [11]. Atmospheric C/O ratios could potentially be a footprint of where and how planets formed in the protoplanetary disks.

2.3. *Characterization of host stars and star–planet interactions*

The exoplanets atmospheric characterization has become the principal target for exploration, in particular with the technique of transit spectroscopy. The observation of light curves during exoplanets transit with spectrometers has given important results on the composition of exoplanets. Nevertheless, many effects can perturb the data reduction: stellar variability, stellar activity, etc. A recent reevaluation of sodium emission on HD209458b [4, 5] has pointed that the combination of stellar lines with planetary lines, with varying Doppler shift due to a rapid stellar rotation (called Rossiter–McLaughlin effect [12, 13]), can perturb the planetary interpretation of Na or K emission. Similar effects are expected when molecular lines are present in cold stars [14], with corrections to take into account to disentangle stellar and planetary spectra. The stellar activity is another important aspect which begins only to be well enough modelized in order to correct for em e.g. granulation or stellar spot, beyond simple limb darkening models [15]. The accuracy of stellar models for FGK stars gives today an access to correction in transit spectroscopy for most effects, when high resolution stellar spectra are available.

2.4. *The ESA-Ariel mission*

The ESA/Ariel mission [16] scheduled for launch in 2029 is devoted to the transit spectroscopy of a representative sample of a thousand exoplanets from temperate Super-Earths to Giant planets. Its main objective is to answer to fundamental questions about planet formation and evolution in a statistical frame, and to put in perspective the question about the condition of the emergence of life. The Ariel mission has been build after the phase A study of the ECHO mission [17]. It is a 1 m class space telescope devoted to the observation by spectroscopy of transiting exoplanets, between 1.1 and 7.8 μm with access to a large number of molecular bands present in planetary atmospheres (e.g. H_2O, CH_4, CO, NH_3, etc.) By observing a known sample of transit exoplanets, Ariel will focus on the transit observation from one planet to the other with agility. The sample target reference list is therefore a major program element to be built in advance. The observation strategy is built on a four Tier approach. Tier 1 aims at observing the whole Ariel sample (~1000 planets) by transit to detect which planets have a cloud-free, H_2-dominated atmosphere and which planets have a cloudy of secondary atmosphere. Tier 2 consists in an atmospheric characterisation by transits and eclipses of ~500 exoplanets to mesure chemical abundances, clouds and thermal structure. Tier 3 is a detailed atmospheric analysis of ~50 planets, cumulating many transits/eclipses. Tier 4 is dediacted to additional science and to phase curves. ~40 planets will be observed by phase curves to map the thermal structure, clouds and chemical composition and to constrain the atmospheric dynamics [18].

The Ariel mission relies on the observation of planetary transit of a large sample of planets. An optimization of the mission process relies on a good knowledge of ephemeris. Many targets are observed from previous mission, especially TESS, and a growing uncertainty with time of the ephemeris accuracy has to be compensated. A program of ground-based observations has been coordinated [19] with the participation of world-wide consortium of observers on small telescopes to update and verify the ephemeris of the Ariel targets.

3. Models for exoplanetary atmospheres

3.1. *Description of 1D/3D atmospheric models*

Atmospheric models are now essential tools for interpreting observations of exoplanetary atmospheres. Many scientific teams around the world have over the past 30 years been developing atmospheric models for exoplanets with different degrees of complexity. These models include key physical/chemical processes ruling planetary atmospheres. A hierarchy of models is available, from simple 1D models, which can be very efficient for simulating observational spectra and for atmospheric retrieval, to complex 3D Global Climate Model (GCM), which are necessary to investigate the atmospheric dynamics of exoplanets. As much as possible, the processes simulated by the atmospheric models are based on universal physical/chemical equations. The ultimate goal is to build virtual planets able to reproduce and predict all the available observations [20]. Historically, the development of atmospheric models for exoplanets started before the detection of the first exoplanet around a Sun-like star [21]. One of the first and still one of the most famous models was developed by Kasting to determine the limits of the habitable zone

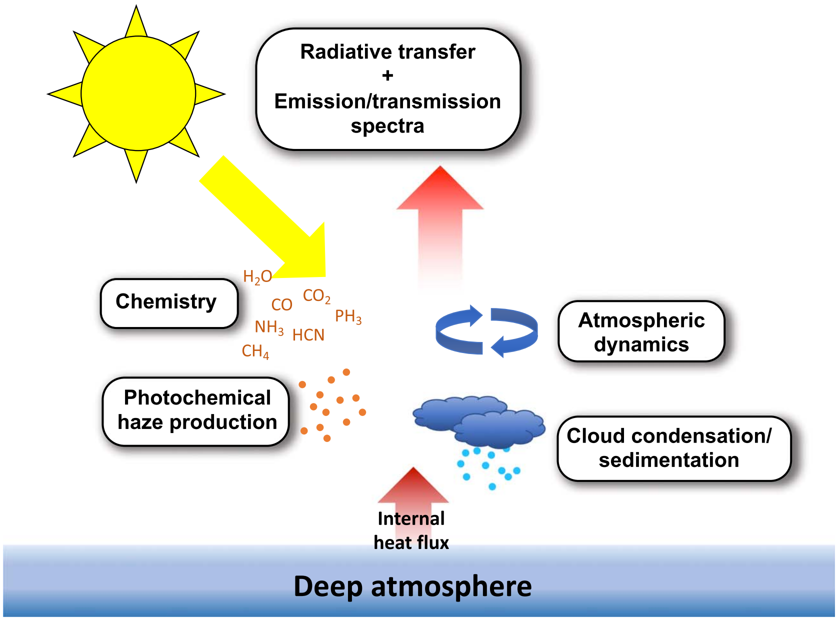

Figure 1. Illustration of the different processes included in a 1D or 3D atmospheric model for gaseous exoplanets.

for different stellar types [22]. The exoplanet community has naturally benefited from developments of atmospheric models for the Earth and solar system planets. It has also strongly benefited from developments from the stellar/brown dwarf community, especially as the first observed exoplanets were hot giant planets. The main processes included in atmospheric models are the radiative transfer, atmospheric dynamics, the chemistry, the cloud/haze formation (see Figure 1).

3.1.1. *Radiative transfer*

The radiative transfer of stellar and thermal radiation is a central element of all atmospheric models for exoplanets. It allows us to compute the heating/cooling rate in the atmosphere, and thus the thermal structure, as well as spectra (in emission, reflection and transmission). For exoplanets, atmospheric opacities in the visible and the infrared includes:

- Molecular lines which correspond to transitions between electronic, rotational, vibrational and roto-vibrational energy levels. A typical planetary spectrum is composed of billions of lines. Beyond the absorption in the visible wavelengths range by atomic sodium and potassium in the NaI and KI doublet, the main source of opacity for gaseous exoplanets are molecules as H_2O, CH_4, CO, NH_3, CO_2, PH_3, VO, TiO Na and K.
- Continuum which varies slowly with wavelength. It can be produced by the contributions of all molecular line far wings. The line profiles far from the center are generally not well known and experimental data are essential to determine the continuum. Continuum can also be produced by collision-induced absorptions (CIA), which correspond to the formation of transitory states with a dipole moment when two molecules collide. This process is fundamental for atmospheres mostly composed of non-dipolar molecules,

such as H_2, N_2 and O_2. H_2–H_2 CIA are one of the main opacities at high pressure ($P > 1$ bar) for gaseous exoplanets.
- Finally, cloud/haze particles produce a continuum opacity for both absorption and scattering.

The most accurate atmospheric models use line-by-line radiative transfer codes, which allows to spectrally resolve each molecular line and to generate spectra at high resolution (e.g. $R = \lambda/\Delta\lambda \sim 10^5$), similar to the resolution of high-resolution spectrograph (e.g. VLT-CRIRES). However, these models are very slow and are generally limited to the calculation of spectra for a given temperature/composition profile. For self-consistent 1D models computing the thermal structure and for 3D models, faster methods are used, as the correlated-k method. In this method, the spectrum is divided into large spectral bands. In a band, the line intensities are reorganized as a smooth distribution, which can be easily fitted with a few points and for which the radiative transfer as monochromatic is applied. The correlated-k method is very fast and quite accurate. The mixing of k-coefficients for a gas mixture is possible, and online tools allow to generate grids of k-coefficients for different atmospheric composition [23].

3.1.2. *Dynamics*

Atmospheric dynamics includes the large-scale circulation as well as more localized atmospheric motions such as gravity waves, convection and turbulence. It is responsible for redistributing stellar energy absorbed in the atmosphere. Planets in our Solar System have relatively small equator-pole and day-night thermal contrasts, contrary to strongly irradiated exoplanets which should belong to different climate regimes. These planets are likely tidally-locked with a synchronous rotation and a permanent dayside/nightside. The strong thermal contrast drives the atmospheric circulation, leading in most cases to the development of equatorial superrotation jets which redistribute heat from the dayside to the nightside. The radiative timescale (defined as the characteristic time of radiative cooling) and the advective timescale (defined as the characteristic time of horizontal wind transport) can be of the same order, allowing us to probe the atmospheric dynamics by measuring the thermal structure and heat redistribution through thermal phase curves. Tidal locking might also affect temperate terrestrial planets in the Habitable Zone of low-mass stars. The circulation regime on these planets could modify the cloud distribution and consequently the cloud radiative effects (albedo cooling effect and greenhouse warming effect), with implications on the limits of the Habitable Zone [24, 25]. 3D GCMs are necessary tools to study the atmospheric circulation on exoplanets and its observational impacts. These models solve the atmospheric fluid equations in a rotating sphere. Depending on GCMs, different assumptions are made (e.g. hydrostatic or non-hydrostatic, shallow or deep atmosphere) and different numerical solvers and grids (e.g. finite-differences or spectral model, latitude-longitude grid or icosahedral grid) are used. 3D simulations are computationally time-consuming, thus the parameter exploration (i.e. the atmospheric chemical composition) is generally limited.

3.1.3. *Chemistry*

The large range of temperature and irradiation of exoplanetary atmospheres covers different regimes where the chemical composition can be at chemical equilibrium (when the concentration of chemical species have reached conditions for no further changes with forward reaction rates equal to reverse reaction rates) or at chemical disequilibrium. The latter relies on the kinetics of chemical reactions and can be due to vertical/horizontal mixing in the atmosphere, UV photolysis, impacts or other processes. The composition at chemical equilibrium can be relatively easily computed in atmospheric models by minimizing the Gibbs energy for each vertical level. However, the range of validity of models only based on chemical equilibrium is very limited. More accurate models include non-equilibrium chemistry either by using parameterizations of the quenching level due to vertical mixing [26] or by solving individual reactions of a chemical network. The development of reduced chemical networks, selecting a limited number of key reactions, allows their implementation in 3D models [27].

3.1.4. *Aerosols*

One of the main discoveries on exoplanetary atmospheres was to realize that most exoplanets are cloudy or hazy. These particles produce flat and featureless transit spectra (e.g. [8, 28]) and potentially high reflectivity in secondary eclipses and phase curves [29, 30]. These particles are either: (1) condensate clouds that grow from an atmospheric specie when the partial pressure of the vapor exceeds its saturation vapor pressure (e.g. iron, silicate or water clouds) or (2) photochemical hazes produced by from photochemistry in the atmosphere that results in the formation of involatile solids (e.g. Titan's hazes) [31, 32]. Clouds and hazes can have a major impact on spectra and their radiative effects must be properly taken into account in atmospheric models to simulate climates or to retrieve molecular abundances and thermal structures. A few cloud models include detailed microphysics (e.g. [33, 34]), while most models use fixed particle sizes or crude microphysics. This last approach with 1D models appears sufficient to reproduce at first order the transition between L dwarfs and T dwarfs, likely due to the disappearance of silicate and iron clouds [35]. 3D models predict that clouds preferentially form on the nightside of irradiated exoplanets, warming the planets by their greenhouse effect [36]. The cloud radiative effects are also a key process for the limits of the Habitable Zone (e.g. [25, 37]) with large uncertainties between models.

3.2. *Atmospheric retrieval*

The principle of atmospheric retrieval is to compare the observed spectrum and data to several simulated spectra computed with an atmospheric model. A statistical method is applied to estimate the most likely atmospheric parameters allowing "to fit the data". Atmospheric models are either self-consistent models, as described in the previous part, or parametric models. The former include different physical/chemical processes and are computationally expensive. They can be used for atmospheric retrieval by computing a grid of models and applying after a statistical method (generally minimization of chi2). However, they cannot explore a large parameter space and the best fit can be biased by the physical/chemical processes included in the model (e.g. the treatment of clouds). Parametric model assume simple parametrisations of the temperature and cloud profiles, defined with a few free parameters, and generally constant profiles of molecular abundances. In contrast to self-consistent models, they are very fast to run, can be used to explore a large parameter space, but can allow degenerated or unphysical solutions. Parametric models are ideal for exoplanets for which there still so many unknowns. However, for low-quality data, they can lead to very degenerated solutions.

The full exploration of the parameter space for the atmospheric retrieval of an exoplanet would generally require a huge number of models, not achievable in a reasonable amount of time. This is why statistical methods are used to quickly explore the parameter space, focusing on the regions where are the best fits. Most of retrieval codes are based on a Bayesian approach to explore the parameter space focusing on the best solutions, to derive posterior distributions. The random exploration of the parameter spaces is done either with a Markov chain Monte Carlo (MCMC) or with the method called Nested Sampling.

3.3. *Lessons for atmospheric modelling*

3.3.1. *When models work and do not work*

Our experience of planetary atmospheres in the solar system (Earth, Mars, Venus, Titan, the giant planets and Pluto) teach us that atmospheric models based on universal equations and a limited number of processes can reproduce well planetary climates and spectra. 1D models have been successful to reproduce thermal emission spectra of brown dwarfs and young giant planets obtained from ground-based instruments, validating molecular line lists at high temperatures. Figure 2 illustrates how 1D models can perform well under such conditions. For transiting hot Jupiters, the equatorial superrotation and the offset in thermal phase curves was predicted by 2D/3D models [10] before it was observed with the Spitzer phase curve of HD209458 b [9]. Generally, the main reasons why models fail to reproduce observations are missing physical processes or neglected 3D effects, as for instance H_2 and H_2O dissociation for ultra-hot Jupiters [36] or nightside clouds on hot Jupiters.

3.3.2. *Biases in atmospheric retrievals*

Biases and degeneracies are currently a strong limitation of atmospheric retrievals. There is in particular a degeneracy between the cloud top pressure and molecular abundances in transit spectroscopy leading to large uncertainties in the measurements of atmospheric metallicity [38]. A large spectral range from the visible to the mid-infared of the combinaison of low and high spectral resolution could break this degeneracy. Another degeneracy related to clouds concerns the retrieval of thermal structure of exoplanets. Indeed, clouds and a reduced thermal gradient similarly reduce molecular feature in emission spectra. Cloud effect can be clearly identified by the detection of cloud absorbing bands (e.g. the silicate feature at 10 μm). Here also, a large spectral range as provided by JWST or Ariel could break this degeneracy. Finally, the 3D structure of exoplanet atmospheres, with strong horizontal variations of temperature and chemical species in particular at the terminators [39], or inhomogeneous and time-varying cloud cover [40], is a large source of uncertainties. It shows the need to use a hierarchy of models from 1D retrieval code to 3D GCM to interpret the observations.

3.3.3. *The interest of intercomparison*

Intercomparison between models is an efficient way to reveal biases and uncertainties. Inspired by the Coupled Model Intercomparison Project (CMIP) done by the Earth's climate modelling community, more and more intercomparisons of exoplanet models are performed. They revealed relatively small differences between models concerning the radiative transfer (e.g. [41]) and the atmospheric dynamics for dry atmospheres (e.g. [42]). However, differences become significant when clouds are included, highlighting the importance of cloud radiative feedbacks (e.g. [43]). A large intercomparison program for exoplanet models involving many teams and called CUISINES (Climates Using Interactive Suites of Intercomparisons Nested for Exoplanet Studies) has recently started.

3.3.4. *Future challenges*

A major challenge for exoplanet atmosphere models is to succeed in reaching the true converged state of the atmosphere. 3D simulations showed that the atmospheric dynamics may evolve over 100,000 Earth days [44], same as the thermal structure in the deep atmosphere which is impacted by the circulation [45]. The challenge for 3D modelling is to cover both the short timescales of chemistry/radiation/dynamics and the long timescales of evolution of the thermal structure and winds in the deep atmosphere.

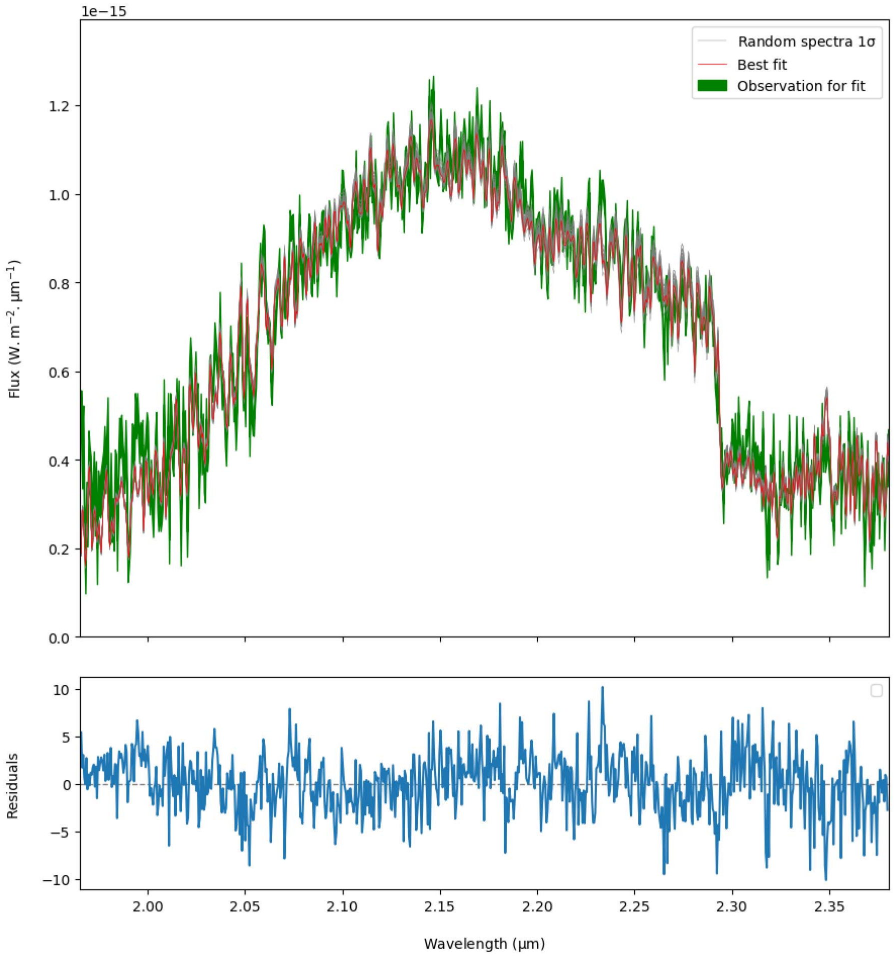

Figure 2. Spectrum of HR8799 b from VLT-SINFONI (in green, R = 5000) compared to the best fit from the Exo-REM model (in red) [35]. The bottom panel shows the residuals between the observations and the model spectrum. Figure from Simon Petrus (personal communication).

Finally, another main challenge related to the previous one is to couple atmospheric models to interior models, to correctly simulate the thermal evolution, chemical composition, radius and spectra. Such models could provide new insights into the interior and formation of exoplanets by simultaneously interpreting spectroscopic measurements and mass/radius measurements.

4. Conclusion and perspectives

The exploration of the Solar System by space remote sensing or in situ probes has renewed the knowledge not only in accuracy, but with a change of perspective: in some sense, Solar System objects have become piece of Earth, and the field of specialists has moved from astronomers to Earth physics (meteorology, geology, geochemistry, etc.) Future years may provide the same change of perspective for exoplanets: even if direct exploration is out of reach due to the distance of exoplanets, a combination of modelling, comparison to Solar System physical processes, and accurate observations by new space or ground-based telescopes will provide a huge amount of data and an expected maturation of the exoplanets science in the next decade.

Conflicts of interest

Authors have no conflict of interest to declare.

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