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INTERIOR-ATMOSPHERE MODELLING OF JWST ROCKY PLANETS

L. Acuña[1], M. Deleuil[1] and O. Mousis[1]

Abstract. Low-mass exoplanets, including rocky planets, might present atmospheres that are massive enough to be detected by JWST in transmission or emission spectroscopy. The first assessment of the observability of their atmosphere is based on their density, which is determined by their bulk composition and irradiance conditions. Interior models can be used in synergy with atmospheric models to get a first estimate of the possible atmospheric properties, including their surface pressure and temperature. In this work, we present a self-consistent interior-atmosphere model that retrieves the planetary internal composition, and generates spectra simultaneously. This allows us to assess the observability and predict spectra based on planetary mass, radius, and optionally, stellar abundances. We apply this model to derive the expected output with JWST for TRAPPIST-1 c and 55 Cnc e, which are two rocky planets proposed for observation that are suspected to have high-molecular weight atmospheres.

Keywords: Planets: interiors, composition, atmospheres. Methods: numerical, statistical. Individual: TRAPPIST-1, 55 Cancri.

1 Introduction

Low-mass exoplanets ($M < 20\ M_{\oplus}$) show two distinctive sub-populations based on their radius: super-Earths, whose radius is $R \simeq 1.3\ R_{\oplus}$, and sub-Neptunes, with radii $R \simeq 2.4\ R_{\oplus}$ (Fulton et al. 2017; Fulton & Petigura 2018). Sub-Neptunes have a volatile-rich composition, with envelopes dominated by H/He, water, or a combination of both (Zeng et al. 2019; Mousis et al. 2020). However, the interior composition of super-Earths is dominated by silicate rocks and Fe. It is still under debate whether super-Earths and Earth-sized planets present thin atmospheres or are bare rocky bodies. Atmospheric characterisation observations will ultimately confirm the presence of an atmosphere in rocky low-mass planets, including emission spectroscopy with the upcoming James Webb Space Telescope (JWST). Nonetheless, interior modelling is necessary to determine whether the density of a planet is compatible with an atmosphere on top of a rocky core within the uncertainties of their observed parameters.

In this work, we introduce a self-consistent interior-atmosphere model that estimates the interior composition and atmospheric properties of low-mass planets given their observed mass and radius. Simultaneously, we take advantage of our atmosphere model to generate emission spectra that can be used to assess the observability of H_2O and CO_2 atmospheres with JWST. In Sect. 2, we describe our interior-atmosphere model. In Sect. 3, we summarize several applications of our modelling framework. Finally, we present our results and conclusions in Sect. 4, which include the generation of spectra for JWST observations for TRAPPIST-1 b and 55 Cancri e.

2 Interior-atmosphere model

Our interior structure model was initially introduced in Brugger et al. (2016, 2017). We consider a one-dimensional grid that represents the planetary radius, along which a set of differential equations are solved to obtain the pressure, $P(r)$; the gravity, $g(r)$, the temperature, $T(r)$; the density, $\rho(r)$, and the enclosed mass, $m(r)$. These equations correspond to hydrostatic equilibrium, Gauss's theorem, an adiabatic temperature gradient, the equation of state and the conservation of mass, respectively. We establish as boundary conditions the pressure and temperature at the surface, and a null gravitational acceleration at the center of the planet.

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[1] Aix-Marseille Univ., CNRS, CNES, LAM, Marseille, France. e-mail: lorena.acuna@lam.fr

The planetary interior is stratified in several layers: a Fe-rich core, a Si-dominated mantle and an water envelope. We adopt the equations of state and thermodynamic properties used in Brugger et al. (2016, 2017) for the core and the mantle. However, the best candidates for atmospheric characterization are highly-irradiated planets that cannot present condensed phases of water on their surfaces. Therefore, we use an equation of state of water at high temperatures and pressures for the water envelope in our interior model, as described in Mousis et al. (2020); Acuña et al. (2021). The input of the interior model are the planetary mass, the core mass fraction (CMF), the water mass fraction (WMF) and the surface temperature and pressure, while their output are the radius and the Fe/Si mole ratio. We couple the interior model with an atmospheric model to calculate the surface temperature and the contribution of the atmosphere to the radius, known as atmospheric thickness (z_{atm}). Our atmospheric model is one-dimensional k-correlated model, based on the model developed by Marcq (2012); Marcq et al. (2017), with updated k-table data for radiative transfer calculations, and an updated equation of state for water at high temperatures and low pressures for the computation of the atmospheric thickness (Acuña et al. in prep). The radiative transfer calculations include the Outgoing Longwave Radiation (OLR), which corresponds to the planetary bolometric emission, and the Bond albedo, which are necessary to estimate the surface conditions at which the atmosphere is in radiative-convective equilibrium. We consider the thermal structure of the atmosphere to be a near-surface dry convective layer, followed by a wet convective layer and an isothermal radiative layer. The interior and the atmosphere are coupled self-consistently by an iterative scheme until the total radius of the planet converges to a constant value (Acuña et al. 2021). For planets whose pressure at the bottom of the atmosphere is below 300 bars, the interior-atmosphere interface corresponds to the planetary surface, while for massive envelopes, the interior and the atmosphere are coupled at a constant pressure of 300 bar.

We implement our forward interior-atmosphere model within a MCMC Bayesian algorithm (Acuña et al. 2021), where the data correspond to the observables: planetary mass, radius and Fe/Si mole ratio. These are used together with the mass, radius and Fe/Si obtained by the forward model to calculate the log-likelihood for a given set of model parameters. This set of model parameters consist of the CMF and the WMF. The MCMC framework enables us to obtain the posterior distribution functions of the non-observable parameters, which are necessary to derive the mean and uncertainties of the CMF, WMF and the atmospheric properties, including the surface pressure.

3 Applications

Our interior-atmosphere model has several applications. The first one is the calculation of core mass fraction and volatile mass fraction trends in planetary systems, as seen in Acuña et al. (2022). We select systems with 5 or more planets whose masses and radii are available. We observe that several of the multiplanetary systems present an increasing water (or volatile) mass fraction gradient with stellar irradiation for the inner planets, whereas the outer planets seem to have an approximately constant volatile content within each system. This trend is particularly clear for the systems TRAPPIST-1 and K2-138. For the systems that present exceptions to this trend, we are able to explain these by either Jeans atmospheric escape, where the planetary core is not massive enough to retain a volatile envelope, or XUV photoevaporation. We are also able to distinguish volatile-rich planets whose envelopes could be dominated by water and other high molecular weight species from those whose atmospheres are H/He-dominated. We also observe that the innermost planets in some of these multiplanetary systems have very high CMFs, presenting a composition similar to that of Mercury. The WMF and CMF trends provide information about the possible formation and evolution processes, such as formation close to icelines and rocklines, and migration.

The second application of our interior-atmosphere model consists of the retrieval of basic atmospheric parameters for H_2O and CO_2 atmospheres given their mass and radius data. The atmospheric parameters we are able to estimate are the surface pressure and temperature, the atmospheric thickness and mass, and the Bond albedo. An example of this is the retrieval we obtain for TRAPPIST-1 b and c in Acuña et al. (2021). The atmospheric thickness is related to the atmospheric scale height, which contributes to the intensity of the spectral features in atmospheric spectra. The third application of our interior-atmosphere model is the generation of emission spectra, which can be used together with noise simulators, such as Pandexo (Batalha et al. 2020), to simulate JWST observations of rocky planets. The input surface pressure and temperature, as well as the pressure-temperature profile for the atmospheric model, are previously estimated with our MCMC interior-atmosphere retrieval. We adapt our atmospheric model to produce emission spectra with a resolution $R \simeq 200$, which is adequate to be the input for the JWST noise simulator.

	H_2O	CO_2
CMF	0.26±0.03	0.25±0.04
VMF	(11.0±5.6) $\times 10^{-6}$	(2.49±2.07) $\times 10^{5}$
P_{surf} [bar]	15±7	35±29
T_{surf} [K]	1293±152	807±102
z_{atm} [km]	203±37	63±12

Table 1. Retrieved core mass fraction (CMF), water mass fraction (WMF), surface pressure and temperature, and atmospheric thickness for TRAPPIST-1 c.

	H_2O
CMF	0.20±0.05
VMF	$(6.7^{+7.4}_{-5.9}) \times 10^{-5}$
P_{surf} [bar]	209±93
T_{surf} [K]	4161±199
z_{atm} [km]	522±46

Table 2. Retrieved core mass fraction (CMF), water mass fraction (WMF), surface pressure and temperature, and atmospheric thickness for 55 Cancri e.

4 JWST observability

For our analysis of TRAPPIST-1 c, we use mass and radius data from Agol et al. (2021), and we estimate its Fe/Si mole ratio as detailed in Acuña et al. (2021). The corresponding surface pressure derived by our analysis is $P_{surf} = 15 \pm 7$ bar (see Table 1). This 1σ confidence interval must be taken carefully since the PDF of the surface pressure does not present a Gaussian distribution shape. An atmospheric surface pressure of zero value is also compatible with the density of TRAPPIST-1 c. Consequently, we can conclude that TRAPPIST-1 c could have a H_2O atmosphere of up to 25 bar of surface pressure, or no atmosphere at all. The molecular weight of CO_2 is higher than that of water vapour, producing a more compressed atmosphere for a similar surface pressure and temperature. In addition, the radiative properties (i.e opacity) of CO_2 yields a lower surface temperature for the same irradiation conditions in comparison to a water-dominated envelope, which contributes to a lower atmospheric thickness. As a consequence, the models with a CO_2 envelope can accommodate a more massive atmosphere for TRAPPIST-1 c than the water models. Fig. 1 shows its spectrum and photometry mean fluxes binned according to MIRI photometric response functions. We observe that for the nIR filters, both atmospheres have very similar fluxes that are compatible within uncertainties, which makes it not possible to distinguish between the two compositions in these wavelengths ($\lambda < 12.8$ μm). For the filters F1500, F1800 and F2100, the mean flux uncertainties of the water and the CO_2 atmospheres do not overlap, being able to tell the difference between compositions. Therefore, observing TRAPPIST-1 c in emission with filter F1500, as proposed by Kreidberg et al. (2021), will enable us to discern the main atmospheric species.

Hu et al. (2021) have proposed to observe 55 Cancri e in emission spectroscopy combining NIRCam F444W filter (3-5 μm), and MIRI's Low Resolution Spectrograph (MIRI LRS; 5-14 μm). We adopt mass and radius data for 55 Cancri e from Bourrier et al. (2018), and host stellar abundances from Luck (2016). A 100% CO_2 envelope is not extended enough to explain its low density, according to our interior modelling. Therefore, we assume a water-dominated atmosphere since its scale height is similar to that of a silicate atmosphere, which has been proposed as its most likely composition (Keles et al. 2022). The water-dominated atmosphere reproduces well the observed mass and radius, which suggests that water as a trace species might be necessary to explain the low density of 55 Cancri e, since a purely dry silicate atmosphere will have a smaller thickness than a CO_2 atmosphere due to their heavier molecular weights. On the other hand, the pure dry silicate bulk could match the low planetary density if the core and the mantle where less dense than that of Earth-like interiors, pointing to a carbon-rich mantle as suggested by Madhusudhan (2012). Fig. 2 shows the complete emission spectrum of 55 Cancri e from 3 to 14 μm. We notice that for wavelengths below 3.5 μm, the noise is too high to distinguish any spectral lines. Nonetheless, the rest of the spectral range of the proposed observations has a low noise level, which makes the spectral features of water easy to identify with JWST in the high-molecular weight atmosphere scenario of 55 Cancri e.

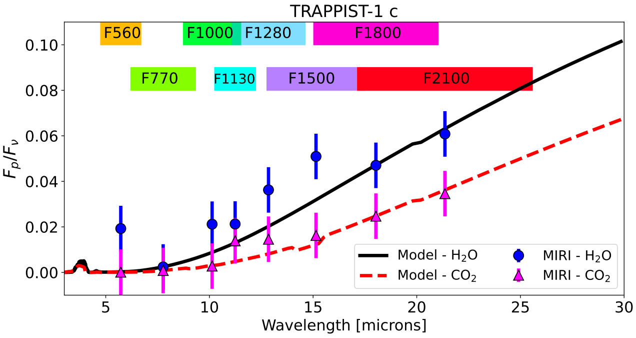

Fig. 1. Simulated emission spectra of TRAPPIST-1 c with MIRI photometric filter mean fluxes for water and CO2 atmospheres

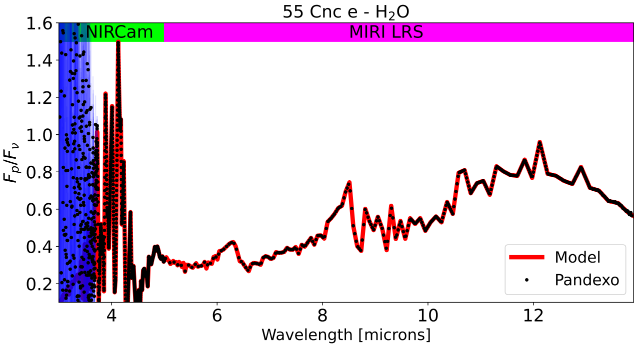

Fig. 2. Simulated emission spectrum for a water-rich atmosphere in 55 Cancri e with NIRCam and MIRI LRS

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References

Acuña, L., Deleuil, Magali, Mousis, Olivier, et al. 2021, A&A, 647, A53

Acuña, L., Lopez, T. A., Morel, T., et al. 2022, A&A, 660, A102

Agol, E., Dorn, C., Grimm, S. L., et al. 2021, The Planetary Science Journal, 2, 1

Batalha, N., Fix, M., Fraine, J., et al. 2020, natashabatalha/PandExo: Release 1.5

Bourrier, Dumusque, X., Dorn, C., et al. 2018, A&A, 619, A1

Brugger, B., Mousis, O., Deleuil, M., & Deschamps, F. 2017, The Astrophysical Journal, 850, 93

Brugger, B., Mousis, O., Deleuil, M., & Lunine, J. I. 2016, The Astrophysical Journal, 831, L16

Fulton, B. J. & Petigura, E. A. 2018, AJ, 156, 264

Fulton, B. J., Petigura, E. A., Howard, A. W., et al. 2017, The Astronomical Journal, 154, 109

Hu, R., Brandeker, A., Damiano, M., et al. 2021, Determining the Atmospheric Composition of the Super-Earth 55 Cancri e, JWST Proposal. Cycle 1, ID. #1952

Keles, E., Mallonn, M., Kitzmann, D., et al. 2022, MNRAS, 513, 1544

Kreidberg, L., Agol, E., Bolmont, E., et al. 2021, Hot Take on a Cool World: Does Trappist-1c Have an Atmosphere?, JWST Proposal. Cycle 1, ID. #2304

Luck, R. E. 2016, The Astronomical Journal, 153, 21

Madhusudhan, N. 2012, The Astrophysical Journal, 758, 36

Marcq, E. 2012, Journal of Geophysical Research: Planets, 117

Marcq, E., Salvador, A., Massol, H., & Davaille, A. 2017, Journal of Geophysical Research (Planets), 122, 1539

Mousis, O., Deleuil, M., Aguichine, A., et al. 2020, The Astrophysical Journal Letters, 896, L22

Zeng, L., Jacobsen, S. B., Sasselov, D. D., et al. 2019, Proceedings of the National Academy of Sciences, 116, 9723