The ARCiS framework for exoplanet atmospheres

Modelling philosophy and retrieval^{★,★★}

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ABSTRACT

Aims. We present ARCiS, a novel code for the analysis of exoplanet transmission and emission spectra. The aim of the modelling framework is to provide a tool able to link observations to physical models of exoplanet atmospheres.

Methods. The modelling philosophy chosen in this paper is to use physical and chemical models to constrain certain parameters while leaving certain parts of the model, where our physical understanding remains limited, free to vary. This approach, in between full physical modelling and full parameterisation, allows us to use the processes we understand well and parameterise those less understood. We implemented a Bayesian retrieval framework and applied it to the transit spectra of a set of ten hot Jupiters. The code contains chemistry and cloud formation and has the option for self-consistent temperature structure computations.

Results. The code presented is fast and flexible enough to be used for retrieval and for target list simulations for JWST or the ESA Ariel missions for example. We present results for the retrieval of elemental abundance ratios using the physical retrieval framework and compare this to results obtained using a parameterised retrieval setup.

Conclusions. We conclude that for most of the targets considered, their elemental abundance ratios cannot be reliably constrained based on the current dataset. We find no significant correlations between different physical parameters. We confirm that planets in our sample with a strong slope in the optical transmission spectrum are those for which we find cloud formation to be most active. Finally, we conclude that with ARCiS we have a computationally efficient tool to analyse exoplanet observations in the context of physical and chemical models.

Key words. methods: numerical – planets and satellites: atmospheres – techniques: spectroscopic

1. Introduction

The study of exoplanet atmospheres is of great interest for putting the rich variety of planets found in the Universe into the context of their formation (e.g. Öberg et al. 2011). The composition of the atmosphere of an exoplanet contains important information on where the atmosphere was accreted, how it evolved, and how it was polluted with solid materials. This information on the dynamics of the planet-forming environment will help us to put the Solar System into a wider context (see also Helling et al. 2014).

Over the past decade, the field of exoplanet research has developed from finding planets and characterising them to first-order into a much more quantitative analysis of the characteristics of exoplanet atmospheres. For a large fraction of this effort, the workhorse has been HST WFC3, which provides a great window on the presence of water vapour (e.g. Tsiaras et al. 2018, for an example on the current state of the art). Future instrumentation, most notably the instruments on board the *James Webb Space Telescope* (JWST), will provide us with a much more in-depth view of the content of exoplanet atmospheres.

The wavelength coverage of JWST extends into the mid-infrared, allowing us to probe solid state features of proposed cloud materials (see e.g. Wakeford & Sing 2015; Mollière et al. 2017).

Analysis of the rich data that are expected in the near future calls for robust analysis tools. These tools have to transform the observational data and attached uncertainties into characteristics of the atmosphere. So-called retrieval methods are needed in order to obtain a set of atmospheric parameters from observed exoplanet spectra (see e.g. Mollière et al. 2019; Fisher & Heng 2018; Barstow et al. 2017; Waldmann et al. 2015; Line et al. 2013; Benneke & Seager 2012; Madhusudhan & Seager 2009). The meaning of the term retrieval is often debated in the context of the difference between retrieval and model fitting. Classical retrieval methods for atmospheres come from the analysis of Solar System objects and Earth observations. Here, the process is used to directly obtain the likelihood distribution of (a set of) parameter(s) with a minimum number of assumptions on the underlying physical system while employing relatively well-known and constrained priors. For example, for the Earth this is easily done since we have exquisite datasets that allow for detailed retrieval of molecular abundances. This is different for the case of exoplanets where we have to explore a very large parameter space, rely on little prior knowledge, and deal with limited observational data. Many studies in the literature on exoplanet retrieval focus on figuring out the required level of

* Numerical implementations of some of the modules presented in this paper can be found at <http://www.exoclouds.com>.

** All data used and created in this paper are available online at <https://zenodo.org/record/3964430>

Fig. 1. Schematic layout of the modelling chain.

complexity – in the form of for example clouds (see e.g. Barstow et al. 2017) or 3D structure of the planet (Caldas et al. 2019) – to reliably retrieve atmospheric information.

In this paper we present a new modelling framework in the form of the ARCIS code (ARTful modelling Code for exoplanet Science). We aim to provide a framework which is both fast and flexible enough to allow robust retrieval methods to be used. Such a retrieval framework that can take into account constraints on physics and chemistry of the atmosphere in a non-parameterised manner is needed to (i) gain insight into the physical and chemical processes like cloud formation, and (ii) make sure that our results are not biased by oversimplified assumptions on the structure of the atmosphere. The idea behind this is not new in the literature and is a generalisation, with additional physical processes, of what could be referred to as chemically consistent retrieval (see e.g. Oreshenko et al. 2017). In Ormel & Min (2019), we introduced a physical transport model for the vapour and condensate species. Here, we add chemical processes to further constrain the molecular abundances (Woitke et al. 2018) and different cloud species to make the code applicable to a wider variety of environments.

In Sect. 2 we describe the modelling philosophy and setup as well as the retrieval part. We apply the retrieval part of the code to the transit spectra of ten exoplanets in Sect. 3.3. We discuss the results and conclude in Sect. 5.

2. Modelling setup

The modelling in the ARCIS (ARTful modelling Code for exoplanet Science) framework aims at using physical parameters from planet formation and evolution to predict observable quantities. Furthermore, we aim to develop a framework with a mild computational load so that robust retrieval algorithms can be employed to link these parameters to observations. The modelling chain is schematically outlined in Fig. 1 and described briefly below. We mainly refer the reader to the relevant papers discussing the various modules in more detail. However, we note

that the concepts for most of the modules are under continuous development.

2.1. Atomic abundances

Setting up an exoplanet atmosphere starts from the abundances of the atoms that form the molecules and condensed species in the atmosphere. The abundances of these elements can, in principle, be predicted from the theory of planet formation and evolution (e.g. Öberg et al. 2011). In many studies the oxygen and/or carbon abundances are scaled with respect to solar values to obtain different chemical conditions. The C/O ratio is one of the most important parameters determining the gas phase chemistry. However, in this paper we also wish to include cloud formation. For this, the ratios of other elements are also important.

In this paper, we consider the ratios C/O, Si/O, and N/O. We start from the Solar abundances as derived by Asplund et al. (2009). First, for C/O ratios above Solar we adjust the oxygen abundance (while keeping C at Solar abundances), and for ratios below Solar we adjust the carbon abundance (while keeping O at Solar abundances). We then adjust the nitrogen abundance to match the N/O abundance. All other elements are scaled with the same value such that we match the Si/O abundance.

After the relative abundances of all elements heavier than He are computed using the above scheme, we scale the H and He abundances with the metallicity parameter, $[Z]$. In our definition of the metallicity this is the added number density of all elements heavier than He divided by the added number density of H and He:

$$[Z] = \log_{10} \left[\left(\frac{\sum_{i \neq \text{H, He}} X_i}{\sum_{i = \text{H, He}} X_i} \right) \cdot \left(\frac{\sum_{i = \text{H, He}} X_i}{\sum_{i \neq \text{H, He}} X_i} \right)_{\text{Solar}} \right], \quad (1)$$

with X_i being the number density of element i .

2.2. Cloud formation

When clouds condense, the element abundances available for the molecules change. Therefore, the first step in our modelling

Table 1. References for the laboratory data for the cloud species.

Solid state species	$\mathcal{A}$	$\mathcal{B}$	Refractive index ref.
(NaAl) _x Mg _y SiO ₃ [s] ^(a)	68 908	38.1	Scott & Duley (1996); Jaeger et al. (1998)
SiO ₂ [s]	69 444	33.1	Gaskell & Johnson (1976)
Fe[s] & FeS[s] ^(b)	48 354	29.2	Henning & Stognienko (1996)
Al ₂ O ₃ [s]	77 365	39.3	Koike et al. (1995)
C[s]	93 646	36.7	Zubko et al. (1996)
SiC[s]	78 462	37.8	Laor & Draine (1993)
TiO ₂ [s] ^(c)	Same as Al ₂ O ₃		Posch et al. (2003)
VO[s] ^(d)	Same as Al ₂ O ₃		Opacities not computed ^(d)

Notes. For the complete list of references for the $\mathcal{A}$ and $\mathcal{B}$ values, see van Lieshout et al. (2016). ^(a)Values for x and y are adjusted to condense all of the Mg and Na. Vapour pressure parameters and opacities are taken to be those for MgSiO₃[s]. ^(b)FeS[s] is only considered for temperatures below 680 K. ^(c)For TiO₂[s] and VO[s] we adopt the values for Al₂O₃[s]. ^(d)For VO[s] no optical constants were available, so VO[s] is ignored in the opacity calculation.

procedure is to compute cloud formation. In many studies, cloud formation is either highly parameterised (see e.g. Barstow et al. 2017) or treated in complete and detailed coupling to the atmospheric chemistry (see e.g. Helling et al. 2008, 2019a; Juncher et al. 2017). Here, we employ a model of intermediate complexity that still catches the essential physics of condensation and transport of the cloud particles. The method is described in Ormel & Min (2019). Here, we expand the method for multiple cloud species for completeness. This is especially important for higher values of the C/O ratio (where it becomes important to include carbon-based cloud species) or high-temperature planets (where it becomes important to include high-temperature condensates). For the saturation vapour pressure of the species we follow van Lieshout et al. (2016),

$$P_V = \exp(-\mathcal{A}/T + \mathcal{B}) \text{ dyn cm}^{-2}, \quad (2)$$

where $\mathcal{A}$ and $\mathcal{B}$ are constants given in Table 1, T is the temperature in K, and P_V is the saturation vapour pressure in dyn cm⁻². At low temperatures, below 680 K, metallic Fe reacts with S to form FeS[s] (Pollack et al. 1994). Therefore, we convert part of the metallic iron below 680 K into FeS[s] such that all S condenses at these temperatures.

When computing which elements are available for the cloud formation we remove gas phase CO. We do this by removing the maximum amount of CO that can form. This implies that when C/O < 1, SiC[s] and C[s] will not condense, while for C/O > 1 all the oxides will not condense. The basic assumption behind this is that CO is a very stable molecule that locks away carbon and oxygen for the formation of solids (see also Helling et al. 2017, for a detailed discussion on cloud formation in carbon and oxygen rich environments).

2.3. Chemistry

For this study we consider equilibrium chemistry for the gas phase. The element abundances are computed after the cloud formation process. Thus, element depletion or enrichment by cloud formation is taken into account. Some of the elements will have been removed by the cloud particles and rained down to deeper layers. This will create elemental abundances that vary throughout the atmosphere (similar to what was shown in e.g. Helling et al. 2008, 2019b). We compute the molecular abundances from this elemental abundance structure using the equilibrium chemistry code GGchem by Woitke et al. (2018).

Table 2. References for the line lists used in the gas opacity computations.

Molecule	Reference
H ₂	HITRAN; Gordon & et al. (2017)
CO, CO ₂	HITEMP; Rothman et al. (2010)
H ₂ O	ExoMol; Polyansky et al. (2018)
C ₂ H ₂	ExoMol; Chubb et al. (in prep.)
CH ₄	ExoMol; Yurchenko et al. (2017)
NH ₃	ExoMol; Coles et al. (2019)
PH ₃	ExoMol; Sousa-Silva et al. (2015)
SiO	ExoMol; Barton et al. (2013)
SO ₂	ExoMol; Underwood et al. (2016)
HCN	ExoMol; Barber et al. (2014)
H ₂ S	ExoMol; Azzam et al. (2016)
Na, K	NIST; Kramida et al. (2013)

In the upper layers of the atmosphere, the chemical timescales may become longer than the mixing timescale; this is where so-called quenching happens. In the uppermost layers, the chemistry may also be affected by UV radiation from the central star (for both effects see e.g. Venot et al. 2012; Kawashima & Ikoma 2018). Both these effects are currently not taken into account in the model but will be the subject of future studies.

2.4. Molecular opacities

Once the molecular abundances are computed, we have to compute the opacities of the molecules. This is done using the available line lists in combination with a method to compute the line profiles. ARCiS uses correlated-k tables for the radiative transfer computations (Lacis & Oinas 1991; Goody et al. 1989). Using accurate line lists is crucial for obtaining the right transmission and emission spectra. The most complete line lists for molecules at high temperatures are provided by the ExoMol project (Tennyson et al. 2016). The problem with this is that the large number of lines makes direct computation of the line profiles numerically cumbersome. A solution for this is given in Min (2017) using a statistical line-sampling technique. However, here we use the standardised precomputed correlated k-tables (at $R = \lambda/\Delta\lambda = 1000$ for the 0.3–50 μm wavelength region) as presented in Chubb et al. (2020) which were computed using the ExoCross program (Yurchenko et al. 2018). The molecules we use in this paper are listed in Table 2 together with the line-list data used. The pressure and temperature broadened profiles for the resonance doublets of Na and K are computed using Allard et al. (2016, 2019).

2.5. Cloud opacities

The opacities of the cloud particles depend on their size, shape, and composition. The composition and average size are computed from the cloud formation procedure, but assumptions are required for the shape. A frequently used assumption is that the particles are homogeneous spheres, so Mie-theory can be applied (Mie 1908). However, even small deviations from a perfect homogeneous sphere can cause large differences with Mie-theory (see e.g. Min et al. 2003). Therefore, here we employ the DHS method (Distribution of Hollow Spheres, Min et al. 2005). This method has been successfully applied to the study of cosmic dust in the interstellar medium (ISM), protoplanetary discs, and the winds of asymptotic giant branch stars (see e.g.

Min et al. 2007; Woitke et al. 2016; Lombaert et al. 2012). The spectroscopic effects of using DHS particles or perfect spheres was investigated by Mollière et al. (2017) showing that the difference could be observable with future telescopes.

The refractive index of homogeneous particles is available through measurements in the laboratory for various species (see also Table 1). The cloud particles we are considering are inhomogeneous; different materials condense on the same particle. For this we can use effective medium theory to construct an effective refractive index from the refractive indices of the various materials (Bohren & Huffman 1983). We use the Bruggeman mixing rule for this (similar to the standard adopted in Woitke et al. 2016).

We note that, like in Ormel & Min (2019), we assume that the nuclei on which the clouds condense have negligible mass and also do not contribute to the opacity of the clouds. These nuclei form what is usually referred to as haze. We realise that the assumption that the only opacity is caused by the condensation species and not by the hazes/nuclei can be significant in certain corners of parameter space. The influence of this assumption will be investigated in a future study.

2.6. Computation of temperature structure

In principle, the temperature structure of the atmosphere can be computed using radiative transfer. This is implemented in the ARCiS code. To compute the temperature structure of the atmosphere we use the Variable Eddington Factor method as also explained in Mollière et al. (2015). The radiative transfer is a strong function of the opacities of the atmosphere. Therefore, we have to iterate cloud formation, chemistry, and computation of the opacities with the radiative transfer to converge to a consistent solution. While currently implemented in the code, we do not use this mode to self-consistently compute the temperature in this paper and leave the discussion of this to a future study. Here we use a parameterised pressure–temperature profile.

2.7. Scattering

The scattered flux is important when considering emission spectra. Scattering can be important for both the thermal flux from the planet itself as well as for scattering of the flux coming in from the central star. Details on the scattering will be presented in a future paper where we will also consider the emission spectra; here we only briefly mention the methods implemented. There are currently two ways to implement scattering in ARCiS. The first is Monte Carlo scattering where the scattered flux is computed by emitting a number of photon packages and tracing them through the atmosphere (see Stolker et al. 2017). The photon packages are emitted as thermal emission from the atmosphere itself as well as from the central star. At random positions, determined by the optical depth travelled by the photon package, the packages interact with the local scatterers and change direction. This iterates until a photon package leaves the system and is collected in one of the bins placed around the planet. This method allows us to take into account the full anisotropic scattering matrix including polarisation effects. However, the drawback is that it can become slow and noisy, and is therefore not suitable for implementation in retrievals. For details on Monte Carlo radiative transfer in exoplanet atmospheres see Stolker et al. (2017) or Lee et al. (2019). The second method we implemented is isotropic scattering using a direct matrix inversion of the scattered flux. Mathematical details on this method

will be presented in a future study. In this paper we only consider transmission spectra. Although scattering can influence the transmission depth in specific cases of for example highly forward scattering clouds (Robinson 2017), we do not include these scattering effects in the computations presented here.

2.8. Computation of transmission and emission spectra

Once the opacity and thermal structure is setup and the contribution of scattered light computed, the transmission and emission spectra can be constructed. For the transmission spectra, this is simply done by computing the optical depth through the atmosphere at different impact parameters and at all wavelengths considered. This way, we compute how much light is blocked by the planet at each wavelength. This can in turn be converted to an effective radius of the planet at each wavelength. For the emission spectra, we have to compute the formal solution of the radiative transfer equation along various rays over the planet. The computation of observables was benchmarked against petitCODE by Ormel & Min (2019). Also, ARCiS was part of the code comparison challenge conducted in the framework of the Ariel mission comparing the forward modelling and retrieval outputs of five different codes (Barstow et al., in prep.). All five codes in this comparison showed excellent agreement on retrieved properties and accompanying uncertainties.

3. Retrieval methods

As mentioned above, there are significant differences between classic retrieval methods designed for Earth observations and retrievals for exoplanet atmospheres. Retrievals for Earth and Solar System atmospheres are often carried out with high signal-to-noise-ratio datasets and a relatively good understanding of the system. This allows for a retrieval approach using relatively well-constrained priors and few assumptions on the physics and chemistry involved. For exoplanets, here we run into some issues. As the data are not as good or complete as those typically available for Earth or Solar System planetary science we always have to make some assumptions. With the data currently available, and also with data expected from future instruments, we cannot obtain the full horizontal and vertical distribution of temperature, density, and molecular abundances. When applied to transmission spectra, the most important commonly used set of assumptions is roughly as follows:

1. 1D spherical geometry;
2. isothermal temperature structure;
3. vertical hydrostatic equilibrium; ideal gas law;
4. homogeneous molecular abundances;
5. grey or smoothly varying cloud opacities.

It is essential to keep in mind that all parameters derived by means of a retrieval method are only valid within the assumptions applied. It is for this reason that many studies in the literature are focussing on pinpointing which assumptions can be made under which circumstances to still get reliable results (see e.g. Rocchetto et al. 2016; MacDonald & Madhusudhan 2017a; Changeat et al. 2019; Caldas et al. 2019). Many of these assumptions can be debated, meaning also the outcome of the retrieval in this way is not necessarily the best representation of the actual parameters of the atmosphere and the interpretation in the context of more complex models becomes very important. Also, for future instrumentation it will be necessary to include a more physically correct model description into retrieval models, encompassing for example pressure-dependent molecular

abundances and temperatures. We refer to methods using the above set of assumptions as the classical retrieval method.

3.1. Model constrained retrieval

With the ARCiS code we have the ability to perform the classical retrieval. However, the added physics and chemistry also allow for what we refer to as a model-constrained retrieval method. In principle any set of model assumptions can be made. In this paper we compare the classical retrieval to the model constrained retrieval using the following set of assumptions:

1. 1D spherical geometry;
2. parameterised temperature structure;
3. vertical hydrostatic equilibrium; ideal gas law;
4. molecular abundances from chemical equilibrium;
5. cloud opacities computed from cloud formation.

We note that the number of parameters in the model-constrained retrieval method is usually slightly lower than for the classical retrieval method since the molecular abundances and cloud properties are computed from only a limited set of parameters. For the temperature structure in the retrieval procedure we do not use the radiative transfer iterations but chose to adopt a parameterised structure following [Guillot \(2010\)](#):

$$T^4 = \frac{3T_{\text{int}}^4}{4} \left(\frac{2}{3} + \tau \right) + \frac{3T_{\text{irr}}^4 f_{\text{irr}}}{4} \left[\frac{2}{3} + \frac{1}{\gamma \sqrt{3}} + \left(\frac{\gamma}{\sqrt{3}} - \frac{1}{\gamma \sqrt{3}} \right) e^{-\gamma \tau \sqrt{3}} \right], \quad (3)$$

with T_{int} being the internal temperature of the planet. The irradiation from the host star is computed using $T_{\text{irr}} = T_{\star} (R_{\star}/r_p)^2$ where $T_{\star}$ is the stellar temperature, $R_{\star}$ the stellar radius, and r_p the distance to the host star. Here τ is the optical depth at IR wavelengths, which we compute using a constant value for κ_{IR} , and $\gamma = \kappa_{\text{vis}}/\kappa_{\text{IR}}$ the ratio between the opacity at visual (irradiated) and IR (outgoing) wavelengths. The parameter f_{irr} specifies the distribution of the incoming flux over the planet.

For the sampling of parameter space, we apply the Multi-Nest algorithm ([Feroz & Hobson 2008](#); [Feroz et al. 2009, 2019](#)). This algorithm searches parameter space and iteratively zooms in on the most promising area of parameter space, that is, the area with maximum likelihood. The algorithm provides accurate posterior distributions for all parameters. Usually at least 10^5 model evaluations are needed for a parameter space which has roughly ten dimensions (see following section for more details on which parameters are used).

3.2. Retrieval validation

First we need to validate the retrieval method as implemented in our code. We have already validated the retrieval algorithm in the framework of the Ariel mission, comparing our retrieval outcome to that of four other codes. Here we present a simple test where we use ARCiS to simulate an observed spectrum and subsequently use the retrieval to obtain the input parameters. We generate a planet with the basic properties of HD 189733b. We use an isothermal profile of 1200 K. The atmosphere consists only of H_2O , CH_4 , and NH_3 with volume mixing ratios 10^{-4} , 10^{-5} , and 10^{-6} respectively. The remaining atmosphere consists of H_2 and He in a ratio 0.85/0.15. We add an optically thick grey cloud deck at $P=0.1$ bar. We simulate a spectrum using the observational wavelength points and accompanying currently available uncertainties (see also following section).

Table 3. References for the observations used in this study.

#	Planet	References
1	HD189733b	Pont et al. (2013) McCullough et al. (2014) Sing et al. (2016)
2	HAT-P-12b	Sing et al. (2016)
3	WASP-12b	Sing et al. (2013) Kreidberg et al. (2015) Sing et al. (2016)
4	WASP-6b	Carter et al. (2020)
5	WASP-31b	Sing et al. (2015) Sing et al. (2016)
6	HAT-P-1b	Wakeford et al. (2013) Nikolov et al. (2014)
7	WASP-39b	Fischer et al. (2016) Sing et al. (2016) Wakeford et al. (2018)
8	WASP-19b	Huitson et al. (2013) Sing et al. (2016)
9	HD209458b	Sing et al. (2016)
10	WASP-17b	Sing et al. (2016)

The resulting posterior distributions from the retrieval of this mock spectrum are presented in Fig. 2. The left plot represents the retrieval performed on the exact data points as computed in the forward model, and the right panel shows the results of the retrieval when we apply Gaussian noise to the data with amplitude of the uncertainties in the observations. As can be seen, the input parameters (represented by the red lines) are retrieved consistently.

3.3. Retrieval applied to ten hot Jupiters

In this section we apply the retrieval framework described in Sect. 3 to the transmission spectra from ten hot Jupiters as presented in [Sing et al. \(2016\)](#). For a list of all references to the observations used, please see Table 3. For easy comparison and consistency we use this dataset in full as it can be downloaded from the website of D. Sing¹ with only two exceptions. For WASP-6b we replace the observations with the homogeneously reduced dataset from [Carter et al. \(2020\)](#). For WASP-12b we add the WFC3 spectrum as presented in [Kreidberg et al. \(2015\)](#). This spectrum has a slight offset with respect to the observations in [Sing et al. \(2016\)](#), and so during the retrieval we allow for an additional parameter scaling the WFC3 spectrum to match the remaining observational data. This scaling parameter is not treated in the same way as the other retrieval parameters but is determined for each forward model computed using a linear least square fit determining its optimal value, and therefore is not represented in the Bayesian posterior distributions. We apply both the classical and the constrained retrieval and compare the results.

We use the nested sampling algorithm as described in Sect. 3 for both retrieval setups. Though the molecular opacities were computed at a spectral resolution of $R=300$, for the retrieval the correlated-k tables are remapped onto the observational grid given the spectral width of each observational point. Typically between 7×10^4 and 1.5×10^5 model evaluations were needed

¹ https://pages.jh.edu/%7Edsing3/David_Sing/Spectral_Library.html

Fig. 2. Results from the retrieval validation tests. *Left panel:* posterior distributions when the retrieval is performed on the mock data without applying Gaussian noise to the simulated observations, *right panels:* posterior distributions when Gaussian noise is applied to the simulated observations. Red lines indicate the input values in the forward model. The green contour lines display the 1, 2, and 3σ uncertainties.

for the multi-nest algorithm to converge. One exception to this was the retrieval for HD 189733b which needed 10^6 model runs to converge. These were run on a single desktop computer with eight CPU cores. The classic retrieval method takes on the order of 30 min per target to converge (~ 50 model evaluations per second), while the model constrained retrieval took around 6 h per target (~ 3 model evaluations per second). Exact computation times depend on the CPU model and even differ from model to model depending on the input parameters and choices on atmospheric setup; therefore these numbers should be taken only as a guide to the order of magnitude. The most time-consuming part in the constrained retrieval setup is the computation of cloud structure and opacities consuming together almost 90% of the computation time. Only a small part of the time is spent in the equilibrium chemistry module since the GGchem code used is extremely efficient.

For the classic retrieval method we use seven species in the gas (H_2O , CO , CO_2 , CH_4 , NH_3 , Na, K) and two parameters for the cloud formation (pressure level of the opaque grey cloud deck and the strength of a diffuse Rayleigh scattering haze). Together with the reference radius (defined at 10 bar), the planet $\log g$ value and isothermal temperature of the planet, this results in 12 parameters to retrieve. For the model-constrained retrieval we have four parameters determining the chemistry (C/O, Si/O, N/O and metallicity), four parameters for the temperature structure (T_{int} , f_{irr} , γ and κ_{vis}), and two cloud formation parameters (the diffusion coefficient, K_{zz} , and the nucleation rate, $\dot{\Sigma}$; Ormel & Min 2019). Together with the radius and $\log g$ of the planet this results in 12 parameters to retrieve as well. All parameters are given in Table 4. For the model-constrained retrieval we include the opacities of all molecules given in Table 2.

We ran the model constrained retrieval also with (1) TiO and VO (using the lines lists from McKemmish et al. 2019, 2016), (2) without Na and K, and (3) constraining the value of f_{irr} to be smaller than 0.25. These resulted in slightly different sets of retrieved parameters, all within 2 sigma of each other. The only

notable exception to this is the fit for HD 189733b with restricted f_{irr} . Since for this source we find a temperature which is far above the expected value from the irradiation (i.e. $f_{\text{irr}} \gg 0.25$), the retrieval was pushed into a very different corner of parameter space. The results with unrestricted and restricted values for f_{irr} for the metallicity were different by 7σ , flipping from sub-solar to super-solar metallicity. Fortunately, the results for all other sources were not significantly affected by these changes. Performing the retrieval with slightly varying model constraints and viewing the results of them all allows a robust interpretation. The results presented below and the correlations discussed are found for all four sets of retrieved parameters. Here, we present the results without TiO and VO, with Na and K, and with $0 < f_{\text{irr}} < 0.25$.

In Table 5 we compare the water abundance we find using the classic retrieval to the results found in Pinhas et al. (2019) for the same sources. We note here that we used different data for WASP-6b, WASP-39b, and HAT-P-12b compared to that study. Also, we use a different model setup, especially for the temperature and cloud structure, which can introduce systematic differences in the derived abundances. In the rightmost column of Table 5 we give the difference between the two studies in terms of their deviation in sigma. Here we see that the two studies appear to be statistically consistent (0 to 1 source with more than 2σ difference, 2 to 3 sources between 1 and 2σ , and 6 to 7 sources below 1σ difference).

Interestingly, we find three sources where, using the classic retrieval, we find constraints on the NH_3 abundance: WASP-31b, WASP-39b, and HD209458b. The abundance of NH_3 we find in WASP-31b is in excellent agreement with that found by MacDonald & Madhusudhan (2017b), who also report a tentative detection of nitrogen-bearing species in HD 209458b (see also MacDonald & Madhusudhan 2017a). For most sources, nitrogen chemistry is not yet very well constrained by the current data, but this will change with the additional precision and broader wavelength coverage of JWST and Ariel.

Table 4. Parameters used in our retrievals.

Parameter	Symbol	Range	Prior
Classic retrieval			
Planet radius	R	5σ around lit. value	Flat linear
Planet log(g)	$\log(g)$	5σ around lit. value	Gaussian prior
Atmospheric temperature	T	300–3000 K	Flat linear
Molecular abundances	X_i	10^{-10} –1	Flat log
Cloud pressure	P_{cloud}	10^{-3} – 10^3 bar	Flat log
Rayleigh haze	f_{mix}	10^{-3} – $10^6 \times \text{H}_2$ scattering	Flat log
Constrained retrieval			
Planet radius	R	5σ around lit. value	Flat linear
Planet mass	M	5σ around lit. value	Gaussian prior
Diffusion coefficient	K_{zz}	10^5 – $10^{12} \text{ cm}^2 \text{ s}^{-1}$	Flat log
Nucleation rate	$\dot{\Sigma}$	10^{-17} – $10^{-7} \text{ g cm}^{-2} \text{ s}^{-1}$	Flat log
C/O	C/O	0.1–1.3	Flat linear
Si/O	Si/O	0–0.3	Flat linear
N/O	N/O	0–0.3	Flat linear
Metallicity	[Z]	–1–3	Flat linear
Irradiation parameter	f_{irr}	0–0.25	Flat linear
Internal temperature	T_{int}	10–3000 K	Flat log
Infrared opacity	κ_{IR}	10^{-4} – $10^4 \text{ cm}^2 \text{ g}^{-1}$	Flat log
Visible to IR opacity	γ	10^{-2} – 10^2	Flat log

Table 5. Retrieved values of the H_2O abundance in the classic retrieval as compared to the results from Pinhas et al. (2019).

#	Planet	$\log_{10}[\text{H}_2\text{O}]$ Pinhas et al. (2019)	$\log_{10}[\text{H}_2\text{O}]$ this study	σ difference
1	HD189733b	$-5.04^{+0.46}_{-0.30}$	$-3.29^{+0.57}_{-0.83}$	1.84
2	HAT-P-12b	$-3.91^{+1.01}_{-1.89}$	$-6.09^{+2.07}_{-2.52}$	0.78
3	WASP-12b	$-3.16^{+0.66}_{-0.69}$	$-2.48^{+0.76}_{-1.00}$	0.57
4	WASP-6b	$-6.91^{+1.83}_{-2.07}$	$-3.35^{+0.47}_{-1.17}$	1.64
5	WASP-31b	$-3.97^{+1.01}_{-2.27}$	$-3.27^{+1.44}_{-2.18}$	0.29
6	HAT-P-1b	$-2.72^{+0.42}_{-0.56}$	$-1.23^{+0.78}_{-3.12}$	0.47
7	WASP-39b	$-4.07^{+0.72}_{-0.78}$	$-1.85^{+1.23}_{-0.58}$	2.41
8	WASP-19b	$-3.90^{+0.95}_{-1.16}$	$-2.68^{+1.15}_{-1.60}$	0.66
9	HD209458b	$-4.66^{+0.39}_{-0.30}$	$-4.68^{+0.53}_{-0.20}$	0.03
10	WASP-17b	$-4.04^{+0.91}_{-0.42}$	$-1.99^{+0.75}_{-1.20}$	1.37

3.4. Comparing classic and constrained retrieval results

The water abundance in classic retrieval results is often used as an indicator of either the C/O ratio of the atmosphere or its metallicity as chemical models predict a link between these parameters. Here we can test this assumption by comparing the H_2O abundance as derived from the classic retrieval to the C/O ratio and the metallicity obtained from the model constrained retrieval. In the left panel of Fig. 3 we plot the H_2O mixing ratio as obtained from the classic retrieval versus the C/O ratio obtained from the model-constrained retrieval. We see no significant correlation between these two parameters. The correlation between the water abundance and the metallicity (right panel of Fig. 3) shows a tentative trend whereby sources with high metallicity have a high water abundance. For both the metallicity and

the C/O ratio we conclude (unsurprisingly) that the data used here are not of sufficient quality and quantity to assess the validity of using the water abundance as a tracer for either the C/O ratio or the metallicity. We note that the way in which we defined the carbon and oxygen abundances is an important factor here. For sub-solar C/O ratios, the oxygen abundance is for example only influenced by the metallicity. A better understanding of how the elemental abundances are coupled from the perspective of planet formation would be very helpful here.

We further compare the atmospheric temperatures obtained with both retrieval approaches. In Fig. A.1 we show the pressure temperature structure for the classic (in red) and constrained (in blue) retrieval methods. The local temperatures appear to agree reasonably well within the error contours derived, especially around the pressures that contribute most to the observed spectrum (i.e. around 10^{-1} – 10^{-3} bar). The temperature structure at very low and very high pressures as derived from both retrieval methods is inaccurate and suffers significantly from the assumptions on the shape of the temperature structure (either isothermal or given by Eq. (3)).

The Bayesian algorithm we employ allows the classic and constrained retrieval to be compared in a formal way. The Bayes factor, which is the ratio between the Bayesian evidence of two models, can tell us if one of the two models is significantly preferred over the other (which is the case when $\ln B_{01} > 5$). The number of free parameters is the same between the two models. We find that for all sources, the Bayesian evidence for the classic retrieval is higher than or equal to that of the model-constrained retrieval. However, the difference is only significant – natural logarithm of the Bayes factor $\ln B_{01} > 5$ – for HAT-P-12b, WASP-39b, and HD 209458b. The logarithm of the Bayes factor is given for all sources in Table 6. The relatively large value of $\ln B_{01}$ for HAT-P-12b, WASP-39b, and HD 209458b suggests that for these sources we have enough information to indicate that there might be physical or chemical processes going

Fig. 3. $\log_{10}$ of the water abundance as derived from the classical retrieval plotted vs. the C/O ratio (*left*) and the metallicity (*right*) derived from the constrained retrieval. The annotated numbers correspond to numbers for the planets as given in Table 5.

Table 6. Natural log of the Bayes factor, $\ln B_{01}$, between the classical and constrained retrievals and the retrieved value for K_{zz} in the constrained retrievals.

#	Planet	$\ln B_{01}$	$\log_{10} K_{zz}$
1	HD189733b	2.0	$11.2^{+0.5}_{-1.2}$
2	HAT-P-12b	6.0	$10.7^{+0.9}_{-3.2}$
3	WASP-12b	2.9	$10.0^{+1.2}_{-1.3}$
4	WASP-6b	0.1	$7.6^{+0.8}_{-0.7}$
5	WASP-31b	2.8	$7.6^{+1.8}_{-0.9}$
6	HAT-P-1b	1.1	$7.5^{+1.7}_{-0.9}$
7	WASP-39b	5.7	$6.6^{+0.4}_{-0.3}$
8	WASP-19b	-0.2	$6.1^{+2.0}_{-0.7}$
9	HD209458b	5.1	$5.9^{+0.1}_{-0.2}$
10	WASP-17b	0.4	$5.7^{+0.5}_{-0.4}$

Fig. 4. Metallicity derived using the model-constrained retrieval vs. the mass of the exoplanets considered. Mass of the exoplanets is given in Jupiter masses.

on that are not captured by our constrained retrieval model. For HAT-P-12b, this is already shown in the exceptional value of the C/O ratio in the constrained retrieval and the low H_2O abundance in the classic retrieval. This is partly caused by the lack of a clear water feature in the WFC3 spectrum of this source. Future observations will have to tell us if this is real.

3.5. Model-constrained retrieval results

We analysed the results of the model-constrained retrievals by looking at correlations between the different derived parameters. Due to the large uncertainties on the parameters (caused by the small wavelength coverage of the observations and the large error bars on the data), no significant correlations have been found. Nevertheless, in this section we summarise our retrieval results for a set of ten giant gas planets all treated with the same retrieval method.

In Figs. 4–6 we plot the metallicity, the C/O ratio, and the Si/O ratio versus the mass of the exoplanet. Wakeford et al. (2017) find a correlation between metallicity and mass. We find

Fig. 5. C/O ratio derived using the model-constrained retrieval vs. the mass of the exoplanets considered.

Fig. 6. Si/O ratio derived using the model-constrained retrieval vs. the mass of the exoplanets considered.

that eight of the ten planets are within 2σ of the solar metallicity. The exceptions to this are WASP-17b and HD 209458b. The C/O ratio shows no correlation at all with planet mass. Interestingly, we find one planet with a C/O ratio significantly higher than the solar value (HAT-P-12b), and one with a lower C/O ratio (WASP-39b). We remind the reader here that these two planets also have $\ln B_{01} > 5$ comparing the classic retrieval and the model-constrained retrieval, which indicates that extra caution is needed when interpreting the retrieval results. Finally, the Si/O ratio is poorly constrained by the current dataset. Only WASP-17b seems to be an outlier here with a significantly low Si/O value. We find that overall most planets are consistent with the solar ratio within 2σ . Pinhas et al. (2019) found that most planets show a sub-solar H_2O abundance which can be caused by sub-solar metallicity or super-solar C/O ratio. We confirm the sub-solar O abundance either with high values for C/O or low metallicity. When we look at the so-called corner plots which visualise the posterior distributions of the Bayesian sampling (see Appendix B), we see that for some sources there is a correlation between the C/O and Si/O. This indicates that for these sources the O abundance is constrained and not the abundance ratios with C and Si.

When a planet forms, it accretes mass from different regions in the protoplanetary disc. These different regions have different elemental abundances. It is therefore expected that the abundance ratios can be used as indicators for the formation location. In particular, from formation simulations we may be able to predict correlations between the C/O ratio, the Si/O ratio, and the metallicity of the accreted atmosphere. In Figs. 7 and 8 we plot these parameters as derived from our constrained retrieval. As can be clearly seen, there are no significant correlations present, mostly due to the large uncertainties on the derived parameters. Future observations can be used to reduce these uncertainties and look for correlations between these parameters.

We can also compare our results directly to the spectral index as computed by Sing et al. (2016). In that paper the authors use the spectral index of the transmission spectrum as a direct indicator for clouds. In Fig. 9 we plot the cloud parameters, i.e. the values we derive for the diffusion strength K_{zz} and the nucleation rate $\dot{\Sigma}$, versus the slope of the transmission spectrum $\Delta Z_{UB-LM}/H_{eq}$ as defined in Sing et al. (2016). There is a strong correlation between the slope and the value of K_{zz} . The sources

Fig. 7. Metallicity vs. C/O ratio of the exoplanets considered derived using the model-constrained retrieval.

Fig. 8. Si/O ratio vs. C/O ratio of the exoplanets considered derived using the model-constrained retrieval.

we find that have a high diffusion strength, and thus strong cloud formation, are also the sources flagged by Sing et al. (2016) as cloudy based directly on the observed spectrum. This is evidence in favour of the efficacy of both the observational method in Sing et al. (2016) and the theoretical cloud formation model considered here. However, we do expect extremely cloudy objects to have a flat spectrum and populate the upper left corner of Fig. 9. For the nucleation rate, we do not find a significant correlation. However, this could be due to the large errors on the derived values for the nucleation rate. The values we derive for the nucleation rate are consistent with the range expected from detailed nucleation rate computations using the models from Lee et al. (2018). In the present study, we assume that the nuclei on which the clouds condense contain negligible mass and therefore do not contribute to the opacity (as in Ormel & Min 2019). This is an assumption that can break down for atmospheres with low values of K_{zz} and inefficient coagulation such that the nuclei can accumulate high in the atmosphere and form a haze layer. We leave investigation of the effect of these hazes to a future study.

We made relatively specific choices on the elemental abundance ratios that we include and how to compute the elemental abundances from this. These choices could be debated and

Fig. 9. Values for K_{zz} (left) and $\dot{\Sigma}$ (right) vs. the spectral index as introduced by Sing et al. (2016) for the exoplanets considered.

should preferentially be related to how we expect the elemental abundances to change from planet formation theory. This is a study we are currently conducting. The influence of these choices is beyond the scope of this paper and is expected to become highly relevant as more accurate and complete data become available from future missions (especially JWST). We checked many other correlations between physical properties of the atmosphere and the planet, but none of them turned out to be significant.

4. Predictions for future missions

We can use the results from the model-constrained retrieval to extrapolate into wavelength regions that will become accessible by future missions like JWST and Ariel. The retrieval gives the range of parameters possible within the constraints of the current dataset. We can use these model constraints to estimate the bounds within which we expect the observations with JWST, for example, to fall. For sources where the current dataset is not very constraining, the extrapolated spectra will have a broad range of possibilities. However, for the better constrained sources, we can make a prediction that is better constrained. This is of course under the assumption that our modelling is correct when extrapolated to longer wavelengths. Such an extrapolation depends on the model used to make the retrieval fit.

In Fig. 10 we show the extrapolated spectrum for all planets considered. The blue shaded areas show the 1, 2, and 3 σ confidence intervals for the transmission depth. As can be seen, the region widens for the wavelengths further away from the current observational dataset. However, it is clear that for four planets with high retrieved values for K_{zz} (HAT-P-12b, HD189733b, WASP-12b, WASP-6b), solid state features due to clouds are to be expected around 10 μm . The features visible here are caused by condensate particles of solid state materials, mainly $\text{SiO}_2[\text{s}]$ and $\text{MgSiO}_3[\text{s}]$. We conclude here that for studies of cloud mineralogy, the source HD 189733b is the most promising candidate. We previously mentioned the sensitivity of the HD 189733b fit to small changes in the retrieval setup. In all cases, the mineral features in the JWST predicted spectrum are very significant. HAT-P-12b, WASP-6b, and WASP-12b are other candidates showing cloud mineral features but with much less confidence. For HAT-P-12b, we see that there are two options for the cloud features, carbon-rich or oxygen-rich

clouds, and these can be distinguished spectroscopically in the 10 μm wavelength range. Finally, in the predicted spectrum for WASP-39b, slight hints can be seen for mineral features. However, detection of these requires very high signal-to-noise-ratio spectra, and determining the feasibility of detecting those requires detailed instrument simulations. Overall, our results suggest that cloud mineral features are expected for sources with $\Delta Z_{\text{UB-LM}}/H_{\text{eq}} > 3$.

The retrieval results, and also the extrapolation to other wavelengths, depend on the underlying model assumptions. This is illustrated in Fig. 11, where we show the extrapolation of the retrieval results for the classic retrieval and the model-constrained retrieval into the JWST wavelength range. There are several noticeable differences. First, the classic retrieval does not contain information about the solid state features and therefore logically cannot predict their presence in the mid-infrared. Second, it can be seen that the predictions from the model-constrained retrieval are sometimes better constrained. For example, using the classic retrieval we have no information on the presence of some molecules like CO or CO_2 , and so their abundance could, in this context, be anything. The model-constrained retrieval uses chemical information to predict the abundances of molecules for which no observational constraint can yet be made. Therefore, the prediction in this wavelength range is better constrained. This clearly illustrates the limitations of retrieval in general; a prediction or retrieval result is only valid within the context of the model assumptions. This holds for both classical and model-constrained retrieval.

5. Conclusions

We present ARCIS, the ARTful modelling Code for exoplanet Science. This code contains many physical concepts and can therefore help us couple observations to theory. Even though chemistry and cloud formation are computed from physical concepts, the code is flexible and fast enough to be used in a retrieval framework. The code is applied to an existing dataset of ten transmission spectra for exoplanets. From the retrieval analysis we conclude:

- Neither the metallicity nor the C/O ratio derived from the model-constrained retrieval appear to correlate with the H_2O abundance as derived from the classic retrieval approach using a parameterised homogeneous atmosphere.

Fig. 10. Extrapolated transmission spectrum into the JWST wavelength range for all ten planets considered. The planets are ordered according to the retrieved value for K_{zz} with highest value at the top left and lowest at the bottom right corner. Data points are taken from [Sing et al. \(2016\)](#). The blue shaded regions denote the 1, 2, and 3 σ confidence intervals.

- We find one source that appears to have a C/O ratio significantly higher than solar (HAT-P-12b) and one with a value significantly lower than solar (WASP-39b).
- The atmospheric diffusion strength, which determines the cloud formation efficiency in our model, correlates strongly with the spectral index, $\Delta Z_{UB-LM}/H_{eq}$, for the sources within our sample.
- We predict the presence of mineral features in the JWST spectra of some of the sources. These are the sources which observationally have a spectral index $\Delta Z_{UB-LM}/H_{eq} > 3$. HD 189733b is the most promising of these.

Overall, the ARCIS modelling approach as presented here provides a promising pathway to compare theory and observations in a robust manner. In the future, we will investigate

Fig. 10. continued.

Fig. 11. Extrapolated spectrum into the JWST wavelength range for HD 189733b. Here we compare the extrapolation using the classic retrieval and the model-constrained retrieval. The classic retrieval result is shifted down by 1000 ppm for visual comparison.

incorporating disequilibrium chemistry and establish a physical link between the elemental abundances and the planet formation process.

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Appendix A: Pressure–temperature profiles for all retrieval sources

Here we plot the pressure–temperature profiles obtained from the classical and model-constrained retrievals.

Fig. A.1. Pressure temperature structures for all ten planets considered. The blue area indicates the 1-, 2-, and 3-sigma limits from the model constrained retrieval, while the red areas indicate the structure for the classic retrieval.

Fig. A.1. continued.

Appendix B: Posterior distributions

Fig. B.1. Corner plots for the constrained retrieval for all ten planets considered. The red lines indicate the solar elemental ratios.

HAT-P-12b

Fig. B.1. continued.

WASP-12b

Fig. B.1. continued.

WASP-6b

Fig. B.1. continued.

WASP-31b

Fig. B.1. continued.

HAT-P-1b

Fig. B.1. continued.

WASP-39b

Fig. B.1. continued.

WASP-19b

Fig. B.1. continued.

HD209458b

Fig. B.1. continued.

WASP-17b

Fig. B.1. continued.

HD189733b

Fig. B.2. Corner plots for the classic retrieval for all ten planets considered.

HAT-P-12b

Fig. B.2. continued.

WASP-12b

Fig. B.2. continued.

WASP-6b

Fig. B.2. continued.

WASP-31b

Fig. B.2. continued.

HAT-P-1b

Fig. B.2. continued.

WASP-39b

Fig. B.2. continued.

WASP-19b

Fig. B.2. continued.

HD209458b

Fig. B.2. continued.

WASP-17b

Fig. B.2. continued.