ExoplANETS-A retrieval framework

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This document describes the retrieval framework as will be applied to the dataset from WP2. The retrieval will have several levels of complexity. Levels 1 and 2 are for datasets that only have transmission spectra available. Levels 3 and 4 are for datasets where also eclipse spectra are available. All retrievals for levels 1, 2 and 3 are ran using both ARCiS and TauREx. Level 4 is only ran using ARCiS.

1 Overview

We consider different levels of complexity for the retrieval. We increase the levels of complexity of the underlying forward model by changing

- from free molecular abundances to equilibrium chemistry,
- from isothermal to parameterised pressure-temperature structure,
- from two independent 1D models for transmission and eclipse to one 3D model.

We have chosen to have the clouds parameterised. The wavelength coverage available in the HST and Spitzer datasets do not allow constraining more complex cloud models. For the models using the chemical equilibrium we use the same molecular opacity sources but with the parameters C/O and metallicity to compute their abundances. For the 3D structure we use two different implementations available in TauREx and ARCiS.

1.1 Planet properties

The planet parameters are taken from the target list provided by the Ariel consortium. Here we take the radius and temperature of the central star and the prior for the mass and radius of the planet. The radius of the planet is retrieved using a flat prior. When using ARCiS we retrieve the $\log(g)$ of the planet using a Gaussian prior on the mass of the planet. When using TauREx the $\log(g)$ of the planet is fixed to the value measured from radial velocity.

1.2 Cloud parameterisation

The wavelength coverage of HST and Spitzer do not allow the details of a full cloud model to be retrieved. In stead we use a very simple parameterisation where we have a fully opaque cloud deck below a certain

Table 1: Schematic overview of the number of parameters.

	level 1	level 2	level 3	level 4
Planet setup	2	2	4	2
Isothermal atmosphere	1	1	1	-
TP-profile	-	-	4	4
H_2O, CO_2, CO, CH_4, NH_3	5	-	10	-
Flat cloud & Rayleigh haze	2	2	4	4
Chemistry	-	2	-	2
3D structure	-	-	-	1
Number of parameters	10	7	23	13

level, P_{cloud}, and in addition a Rayleigh scattering haze above that. This haze is implemented by simply adding Rayleigh scattering with an opacity κ_{haze} at 1 μm and a spectral dependance of

$$\kappa = \frac{\kappa_{haze}}{(\lambda[\mu\mathrm{m}])^4} \tag{1}$$

The values of P_{cloud} and κ_{haze} might vary over the face of the planet so in the case where we have either two independent 1D models or one 3D model, we also have multiple values for these parameters. In the TauREx code the implementation of the clouds uses different parameters following the notation of Lee 2013. Here the mixing ratio of Rayleigh scattering haze particles is fitted in stead of their total opacity. In practice this is only a scaling factor different and has no influence on the results.

2 Levels of complexity

2.1 Level 1: parameterised setup for transmission

This will be applied to transmission spectra only.

We use the classic retrieval setup for transmission spectra using parameterised abundances for the molecules. We include opacities for H_2O, CO_2, CO, CH_4, and NH_3. The temperature structure is isothermal and we use the cloud parameterisation as described in Section 1.2. We also include in the setup H_2 and He in the ratio 0.85, 0.15.

Parameters:

- Planet parameters: R_p, $\log(g)$
- Molecular abundances: H_2O, CO_2, CO, CH_4, NH_3
- Temperature: T_p
- Cloud parameters dayside: P_{cloud},
  - ARCiS: κ_{haze}
  - TauREx: $N_{\mathrm{mix,haze}}$

2.2 Level 2: chemical equilibrium for transmission

This will be applied to transmission spectra only.

We use the same framework as level 1 with the exception that the molecular abundances are computed using chemical equilibrium. To parameterise the elemental abundances we use two parameters; C/O and $[Z]$. We include the molecules: H_2O, CO_2, CO, CH_4, NH_3, HCN, TiO, VO, AlO, FeH, OH, C_2H_2, CrH, H_2S, MgO, H^-, Na, K, H_2 and He.

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). This simulated removal of these elements during formation or evolution of the planet.

After the relative abundances of all elements heavier than He are computed using the C/O ratio, 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:

$$[Z] = \log_{10}\left[\left(\frac{\Sigma_{i\neq H,He} X_i}{\Sigma_{i=H,He} X_i}\right) \cdot \left(\frac{\Sigma_{i=H,He} X_i}{\Sigma_{i\neq H,He} X_i}\right)_{\text{Solar}}\right], \tag{2}$$

with X_i being the number density of element i.

We use the ggchem code to compute the chemical equilibrium abundances.

Parameters:

- Planet parameters: R_p, $\log(g)$
- Elemental abundances: C/O, $[Z]$
- Temperature: T_p
- Cloud parameters dayside: P_{cloud},
  - ARCiS: κ_{haze}
  - TauREx: $N_{\text{mix,haze}}$

2.3 Level 3: parameterised setup for eclipse and transmission separate

This will be applied to sources where both transmission and eclipse data is available. We apply the retrieval to both observations independently.

For the terminator region (i.e. when retrieving on the transmission data) we use the setup from the level 1 retrieval.

For the temperature structure at the dayside (i.e. when retrieving on the eclipse data) we adopt a parameterised structure

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

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.

When running the ARCiS code we consider isotropic scattering in the atmosphere. For the albedo of the cloud particles we assume for simplicity that the grey cloud deck is fully absorbing (albedo equal to 0), and the haze is (almost) fully scattering (albedo equal to 0.999). We take the albedo of the haze to be less than 1 for numerical stability.

Within the TauREx code we do not use the parameterised profile above, but in stead use a completely free pressure temperature profile fixed at three pressure points. Comparing these slightly different setups allows us to address the robustness of the derived parameters.

Parameters:

- Planet parameters terminator: R_p, $\log(g)$
- Molecular abundances terminator: H_2O, CO_2, CO, CH_4, NH_3
- Temperature terminator: T_p
- Cloud parameters terminator: P_{cloud}, κ_{haze}
- Planet parameters dayside: R_p, $\log(g)$
- Molecular abundances dayside: H_2O, CO_2, CO, CH_4, NH_3
- Temperature structure dayside:
  - ARCiS: $T_{\rm int}$, $f_{\rm irr}$, $\kappa_{\rm IR}$, γ
  - TauREx: free using 3 point profile
- Cloud parameters dayside: P_{cloud},
  - ARCiS: κ_{haze}
  - TauREx: $N_{\rm mix,haze}$

2.4 Level 4: chemical equilibrium for simultaneous eclipse and transmission

This will be applied to sources where both transmission and eclipse data is available. We apply the retrieval to both observations simulataneously.

Both ARCiS and TauREx use a multiple 1D model setup to simulate a 3D structure. The 1D setup is chosen to be the eclipse retrieval setup of the level 3 retrieval. The difference between the two codes is in how the parameters are allowed to vary across the surface of the planet.

2.4.1 ARCiS

The 3D setup in ARCiS is shaped using a diffusion equation which determines how the energy is spread over the surface of the planet. We compute the f_{irr} parameter from

$$\nabla \cdot \vec{v} f_{irr} - K_{xx} \nabla^2 f_{irr} = S. \tag{4}$$

For simplicity we convert to a unit sphere and dimensionless velocity and diffusion coefficients. We compute diffusion over the surface of a unit sphere assuming the velocity vector is in longitudinal direction. This then translates in spherical coordinates to

$$\frac{v_\Lambda}{\cos\Phi}\frac{\partial f_{irr}}{\partial\Lambda} - \frac{K_{xx}}{\cos\Phi}\frac{\partial}{\partial\Phi}\left(\cos\Phi\frac{\partial f_{irr}}{\partial\Phi}\right) - \frac{K_{xx}}{\cos^2\Phi}\frac{\partial^2 f_{irr}}{\partial\Lambda^2} = S, \tag{5}$$

where the source term is given by

$$S = f_{irr,0}(\cos\Lambda\cos\Phi), \tag{6}$$

on the dayside and

$$S = 0, \tag{7}$$

on the nightside. Here Λ and Φ are the longitude and latitude respectively, $f_{irr,0}$ is basically the efficiency with which the planet absorbs the stellar photons (i.e. it is inversely proportional to the planet albedo). The best parameters to derive when considering emission or phase curve observations is the contrast between the day and the night side and the ratio $\eta = v_\Lambda/K_{xx}$. We use the parameter, $f_{n/d}$ which is the integrated energy at the night side divided by the integrated energy emitted from the day side, as retrieval parameter. For the level 4 retrievals we set the parameter determining the shift of the planet hotspot, $\eta = 0$, since we do not have phase curve information. We adjust the value of K_{xx} such that the given value of the parameter $f_{n/d}$ is reached.

Once f_{irr} is computed over the entire globe of the planet, we have the possibility to make all retrieval parameters a function of f_{irr} and thereby vary them when the local temperature varies. In the level 4 retrievals we only vary the cloud parameters, P_{cloud} and κ_{haze}, linearly with f_{irr}. This results in 4 in stead of 2 parameters (the minimum and maximum values for both P_{cloud} and κ_{haze}). At each location on the planet the temperature structure is computed using Eq. 3 with everywhere the same values for $T_{\rm int}$, $\kappa_{\rm IR}$, and γ.

Parameters:

- Planet parameters: R_p, $\log(g)$
- Elemental abundances: C/O, $[Z]$
- Temperature structure: $T_{\rm int}$, $f_{\rm irr,0}$, $\kappa_{\rm IR}$, γ
- Cloud parameters: $P_{cloud,min}$, $P_{cloud,max}$, $\kappa_{haze,min}$, $\kappa_{haze,max}$
- 3D structure: $f_{n/d}$