Atmospheric models for retrieval and interpretation

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Ecole des Houches, *2022*

20 years of exoplanet atmospheric characterization

- Exoplanet atmospheric observations are now done routinely
- Observations revealed a great diversity of atmospheres, many of them seem cloudy/hazy
- Plenty molecules/atoms detected (H_2O, CO, CH_4, NH_3, HCN, CO_2, C_2H_2, H, He, Na, K, Cr, V, Fe, FeH, TiO, VO, $C^{13}O$)

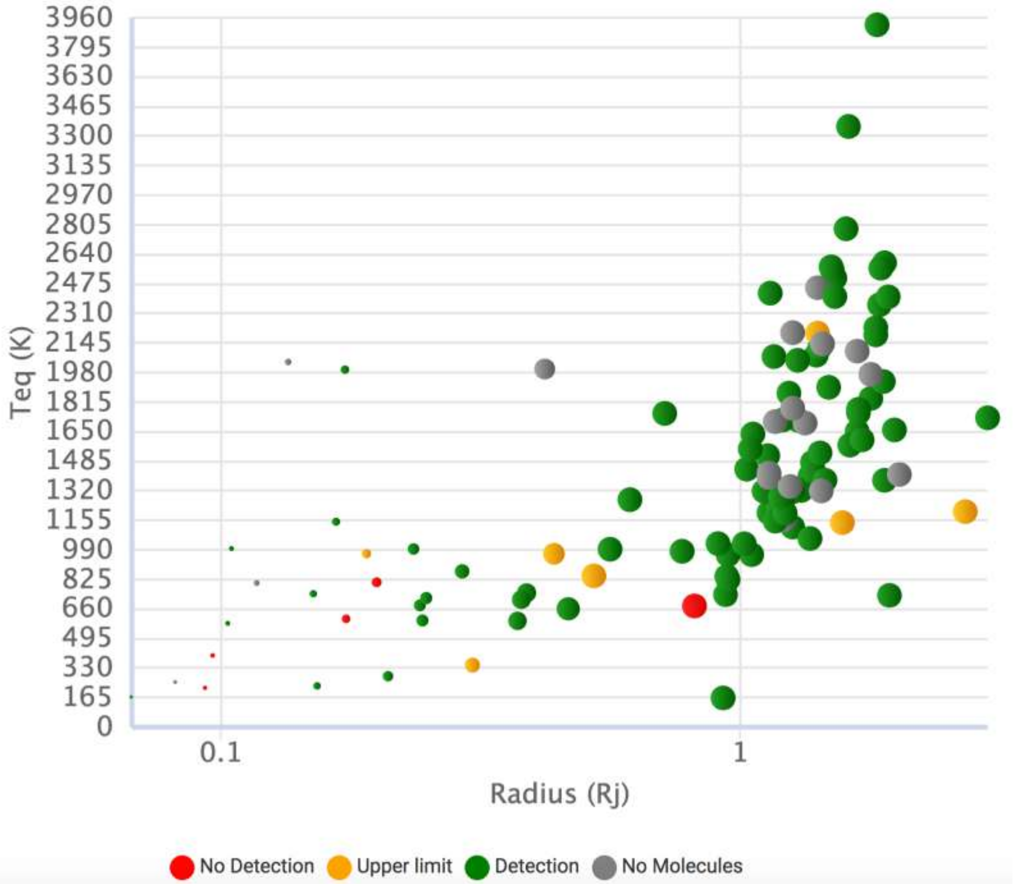
		Properties		Bulk		Ices				Alkalis			Rocks					Isotope
	Planet name	Teq/ Teff (K)	M (M_{Jup})	H	He	H_2O	CO	CH_4	HCN	Na	K	Li	Fe	Mg	Ca	V	Cr	^{13}CO
Transiting planets	KELT-9b	4048	2.88	H									H	H	H			
	WASP-33b	2781	2.1	H		L	L						H		H			
	WASP-189	2641	1.99										H	L		L	L	
	WASP-121b	2359	1.18	H		M				H	H	L	H	H	H	L	L	
	KELT-20b	2255	3.38	H		L				H			H	L	H			
	WASP-76b	2182	0.92			L				H		L	H	L	H	L	L	
	HAT-P-32b	1801	0.58	L	L	L												
	WASP-77Ab	1741	2.29			H	L											L
	WASP-17b	1698	0.78			L				L								
	HD209458 b	1476	0.73	L	L	H	H	L	L	C				C				
	WASP-127b	1401	0.18			L				H	L	L						
	XO-2b	1327	0.566							L	L							
	HAT-P-1b	1322	0.525			L				L								
	WASP-52 b	1299	0.46	L		L				H	L							
	WASP-96b	1286	0.48			L				L								
	HD189733b	1192	1.13		H	H	H		L	H	L							
	WASP-39b	1120	0.28			L				L								
	WASP-6b	1093	0.37			L				H	H							
	WASP-69b	988	0.29		L	L				H								
	HAT-P-12b	957	0.21			L				L								
	HAT-P-18b	848	0.20		L	L												
	HAT-P-11b	829	0.084		M	L												
	WASP-107b	739	0.12		H	L												
	GJ3470b	604	0.043		L	L												
Non Transiting	Tau Bootis b	1636	5.84			C	H											
	HD179949b	1552	0.92			M	L											
	51Peg b	1260	0.46			H	L											
	HD 102195b	1053	0.46			L		L										
Directly Imaged	CQ Lupi b	~2650	25			L	L											
	Beta Pictoris b	~1724	12.9			H	H											
	TYC 8998-760-1b	~1700	14			L	L											L
	HR8799c	~1100	8.1			H	H	C										
	HR8799b	~900	5.8			L	L	C										
	51 Eridiani b	~760	9.1			H		H										

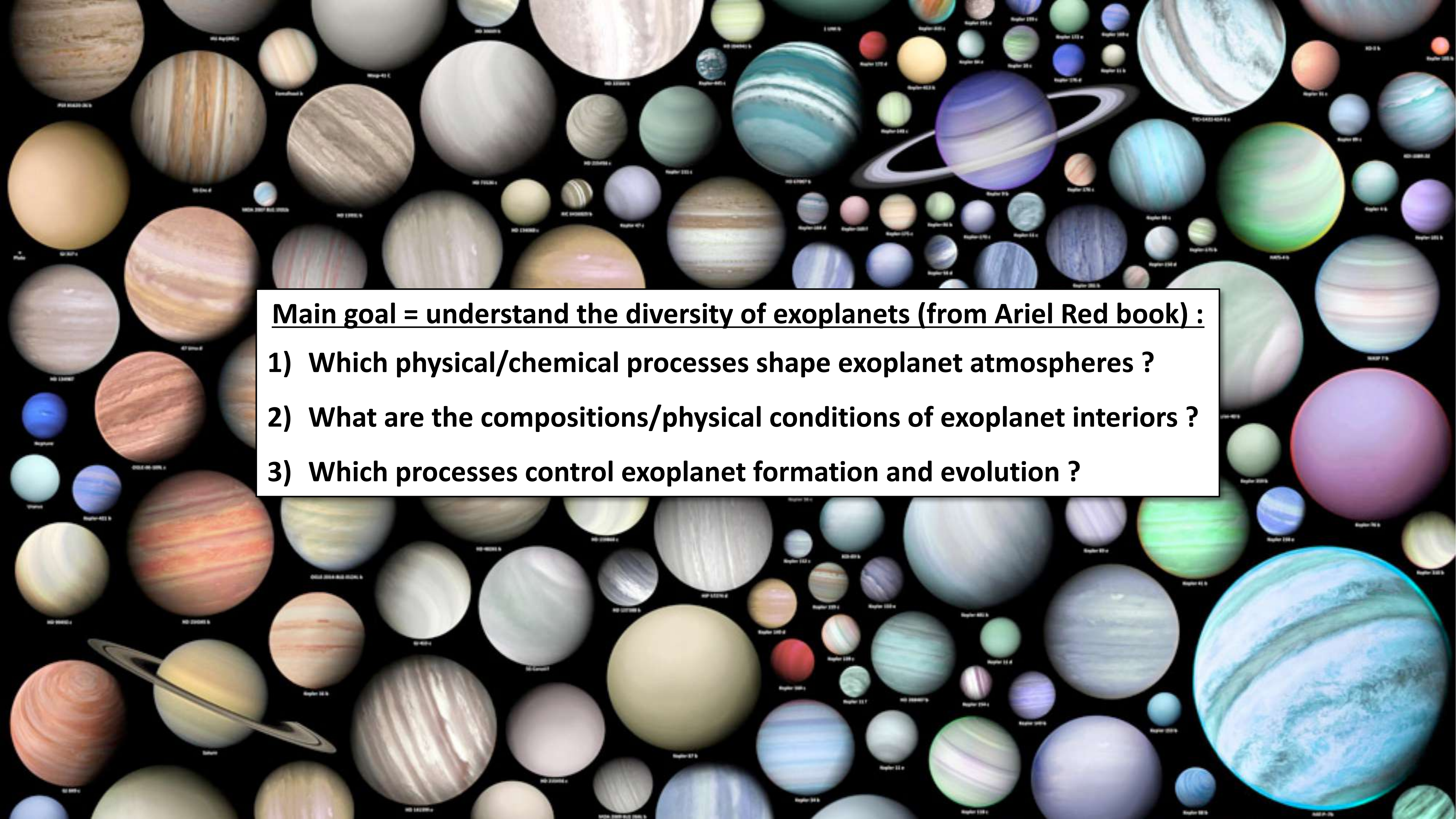
Confidence level:
- High observed by at least 2 instruments
- Medium: observed by one instrument multiple times
- Low: observed once by one instrument
- Controversial

Only planets with at least two different species detected and only species that are detected in at least two planets are presented here. Photometric only detection are discarded. Additional rocks detections (Ti, Sc, Si), ionic species, together with all references are in the full table in appendix.

Guillot et al. 2022

ExoAtmospheres database

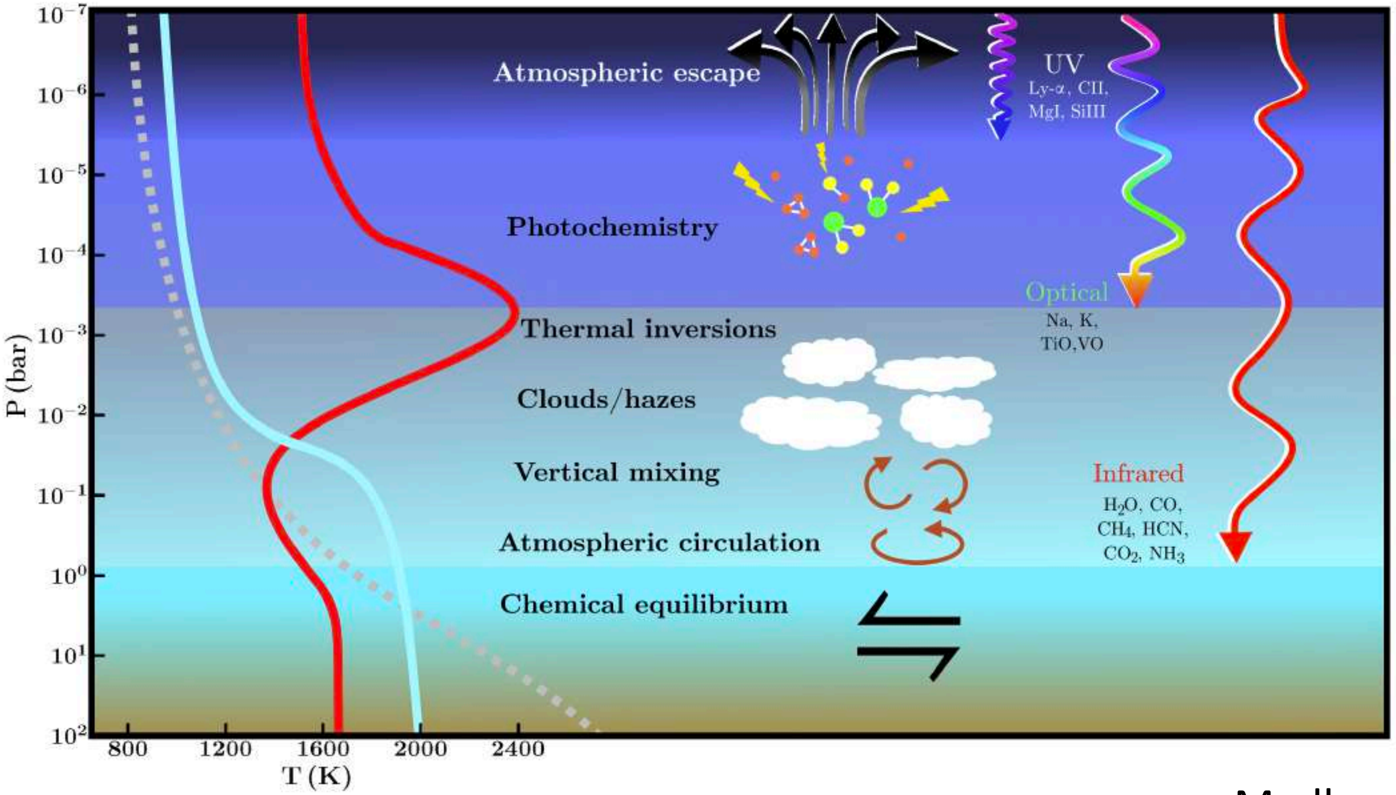




Main goal = understand the diversity of exoplanets (from Ariel Red book) :

1) **Which physical/chemical processes shape exoplanet atmospheres ?**
2) **What are the compositions/physical conditions of exoplanet interiors ?**
3) **Which processes control exoplanet formation and evolution ?**

What is the thermal structure of exoplanets and how is it shaped?

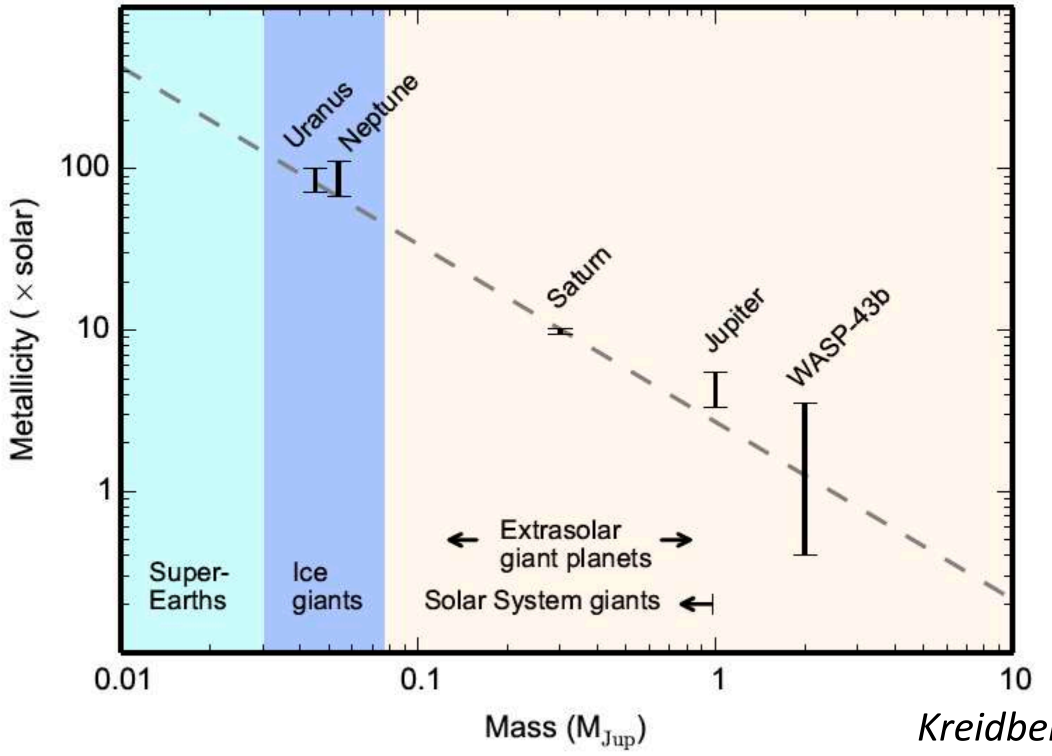


Madhusudhan 2019

- Which planets have a stratospheric thermal inversion ?
- What is the impact of clouds, atmospheric dynamics or fingering convection ?

Atmospheres as a probe of planetary interior and formation

Metallicity = fraction of heavy elements (heavier than H and He)
For Solar System atmospheres, metallicity ≈ $[C]/[C]_{solar}$
For exoplanetary atmospheres, metallicity ≈ $[O]/[O]_{solar}$



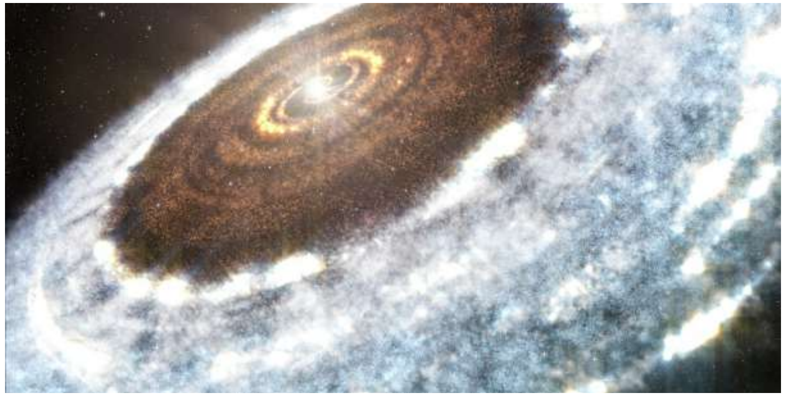
Kreidberg et al. (2015)

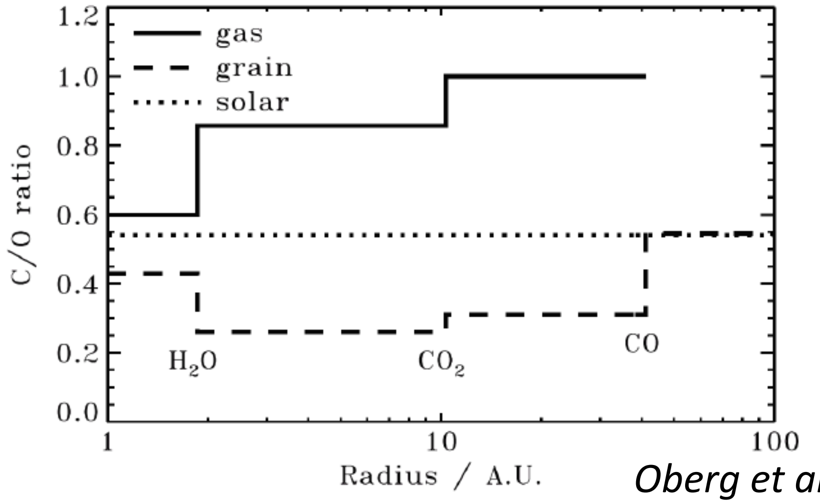
- Metallicity decreases with planetary mass in the Solar System
- Short-period planets formed in-situ should have a relatively low metallicity

→ **Metallicity measurements give constraints on formation and migration mechanisms**

Atmospheres as a probe of planetary interior and formation

$$C/O = \frac{([CO]+[CO_2]+[CH_4])}{([H_2O]+[CO]+2[CO_2])}$$

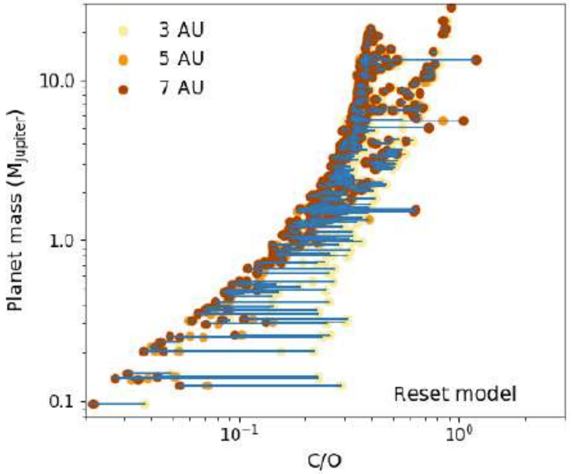




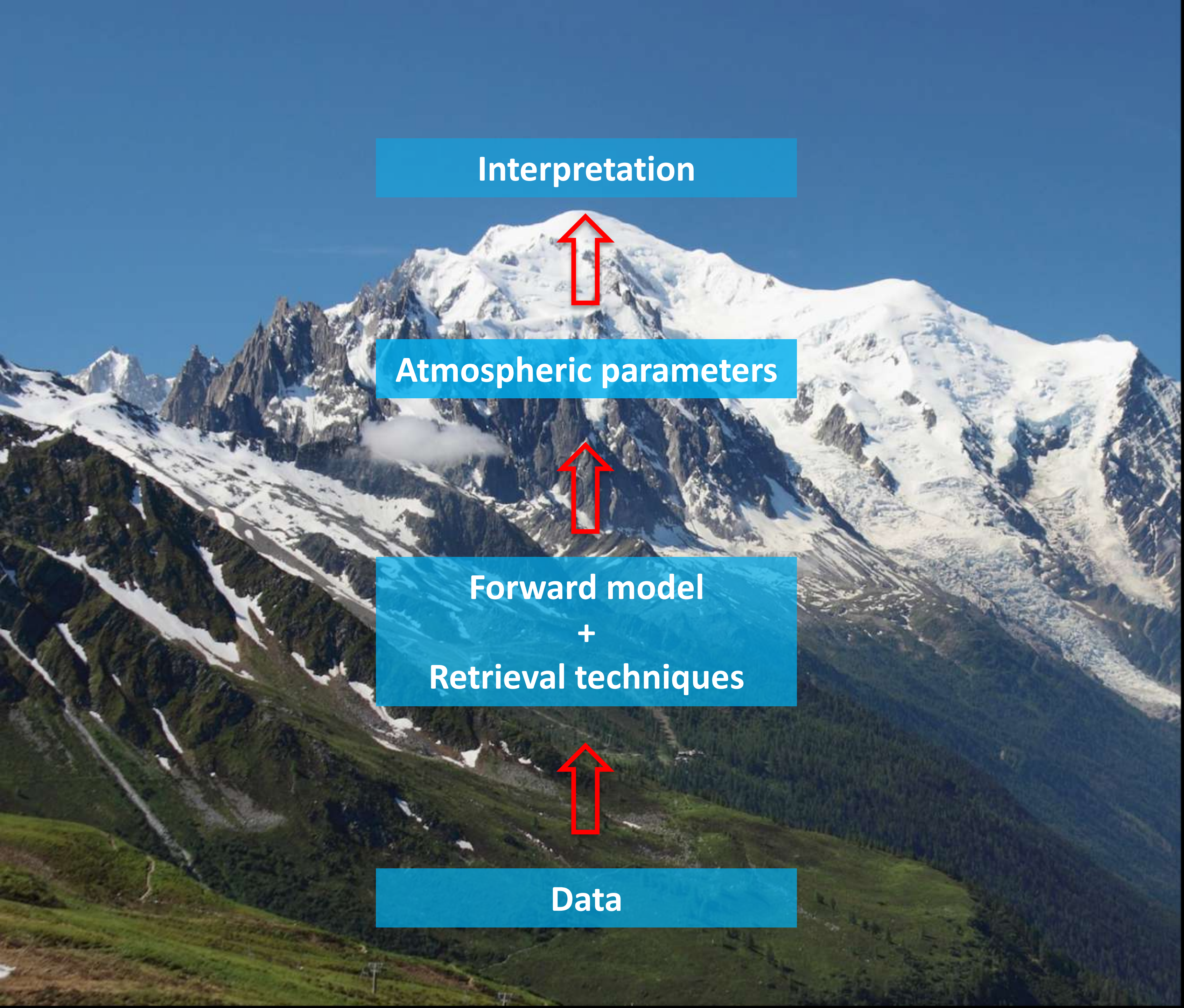
Oberg et al. (2013)

- Atmospheric C/O may depend on where the planet formed
  High C/O => gas accretion
  Low C/O => enrichment by planetesimal
- C/O may decrease for low-mass planets
- The reallity is certainly much more complex

→ **C/O measurements give constraints on formation mechanisms**



Cridland et al. (2020)

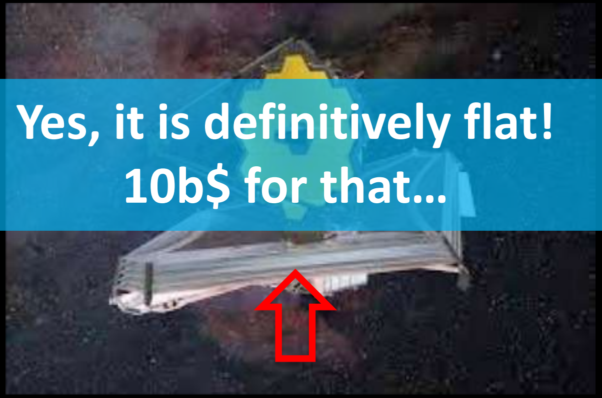


Interpretation

Atmospheric parameters

Forward model
+
Retrieval techniques

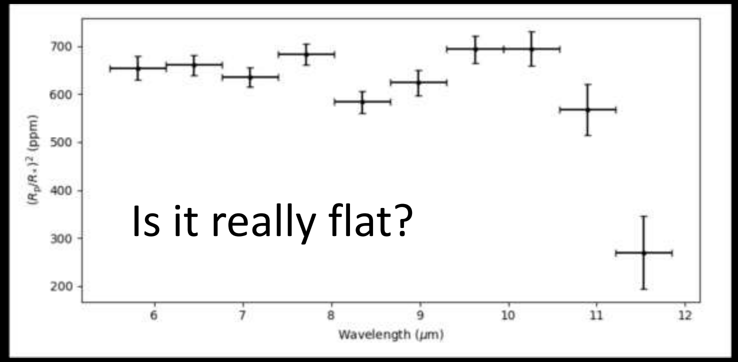
Data



Yes, it is definitively flat!
10b$ for that…

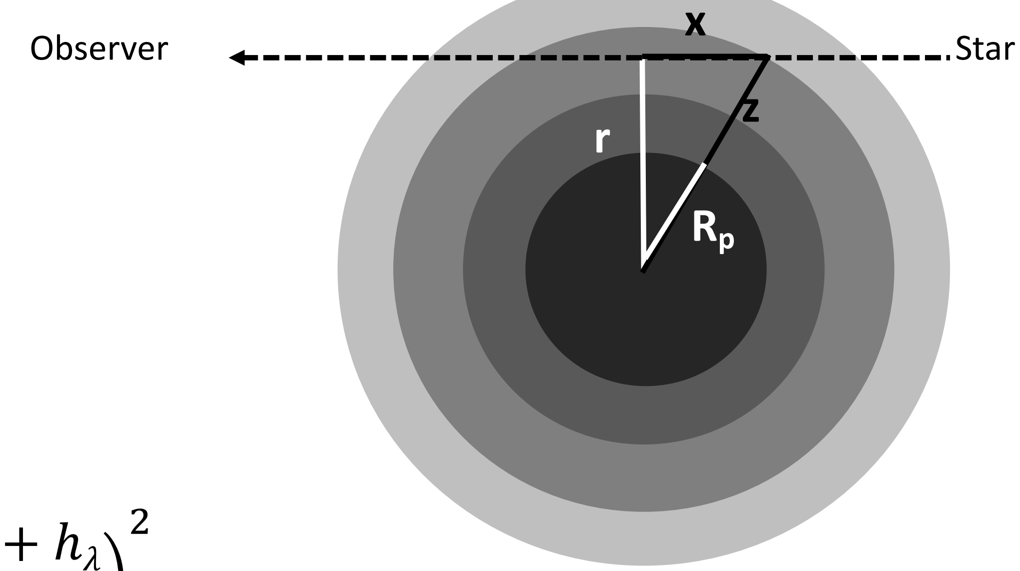
No atmosphere, clouds or high mean molecular mass

e.g. TauREX



1D Forward models

Radiative transfer: transit spectroscopy



Optical depth (cross-section):

$$\tau(r,\lambda) = \sum_i \int_{-\infty}^{+\infty} \sigma_i(\lambda, P, T) n_i(z) dx$$

Transit depth:

$$D(\lambda) = \left(\frac{R_p}{R_\star}\right)^2 + \frac{2}{{R_\star}^2}\int_{R_p}^{R_\star} r\left(1 - e^{-\tau(r,\lambda)}\right)dr = \left(\frac{R_p + h_\lambda}{R_\star}\right)^2$$

Equivalent altitude:

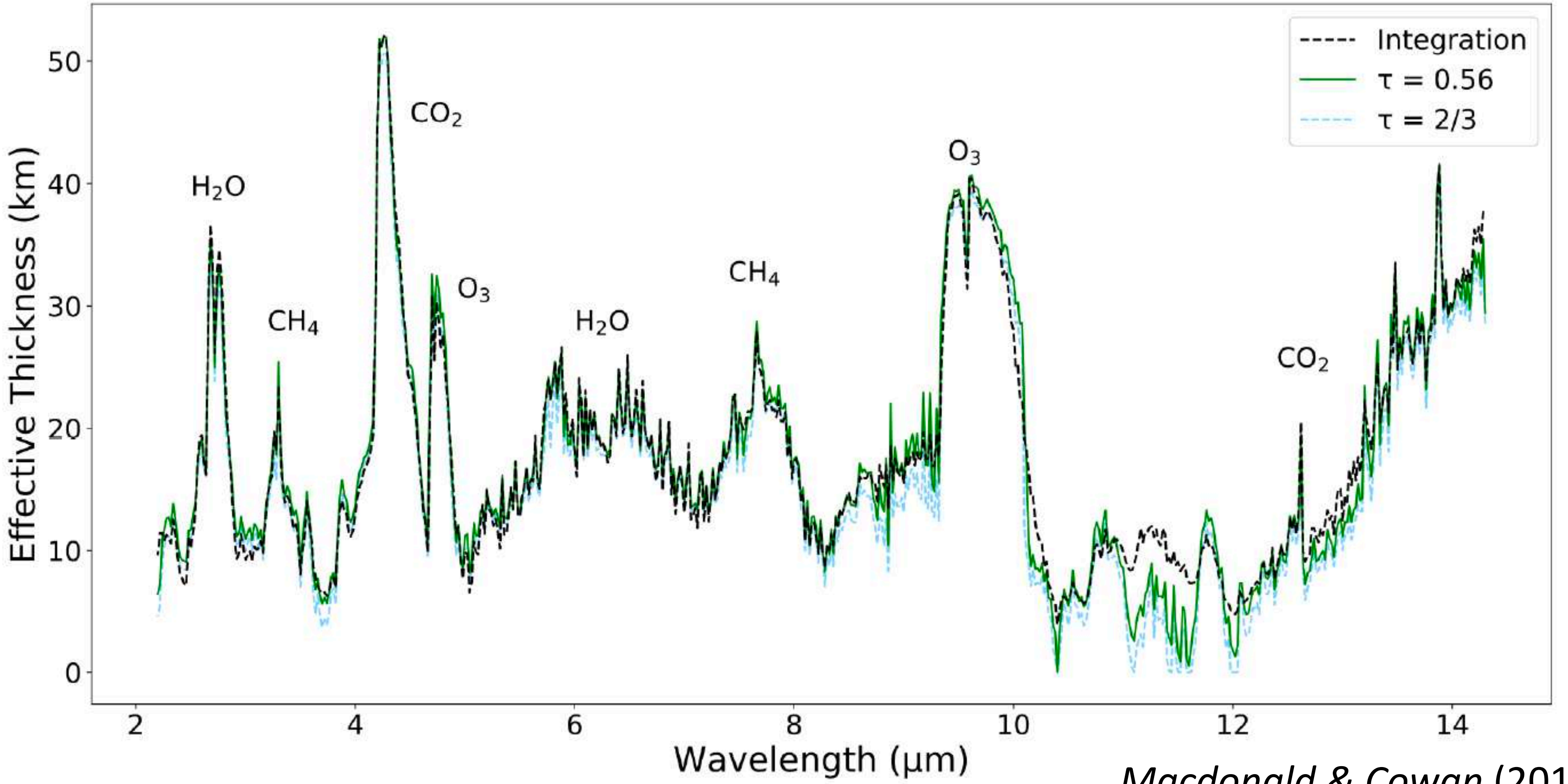
$$\boldsymbol{h_\lambda \approx r(\tau = 0.56) - Rp}$$

see *De Wit & Seager* (2013) and *Macdonald & Cowan* (2019)

1D Forward models

Radiative transfer: transit spectroscopy

Synthetic Earth's transit spectrum

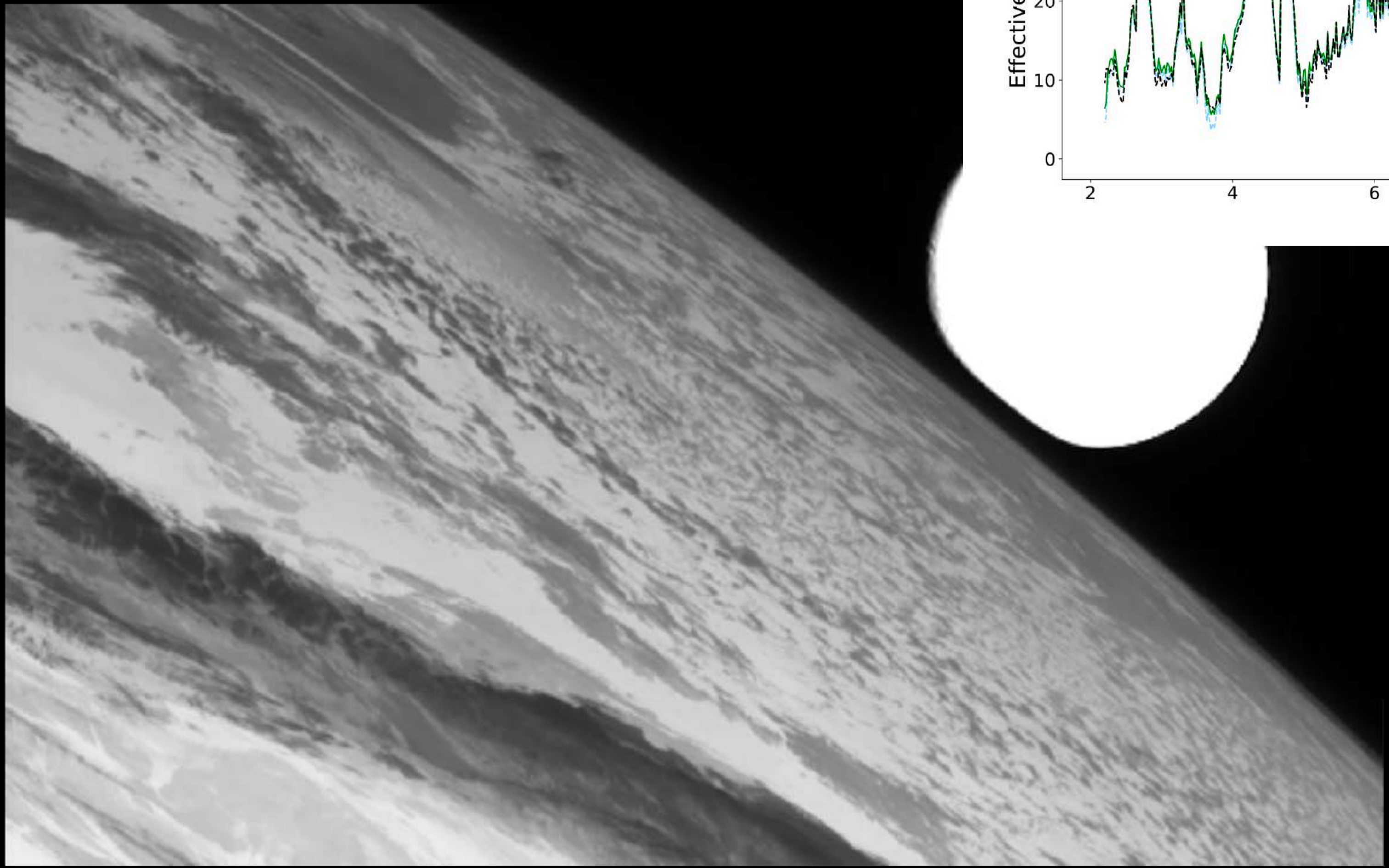


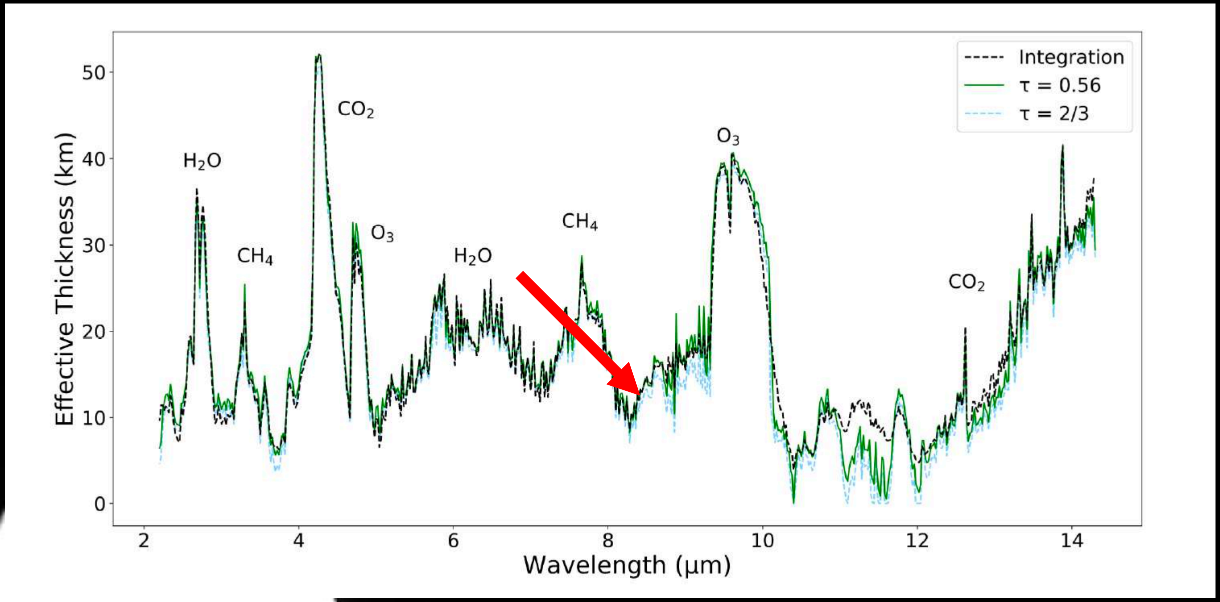
Macdonald & Cowan (2019)

Real color

Credit: Himawary/Simon Proud/Vivien Parmentier

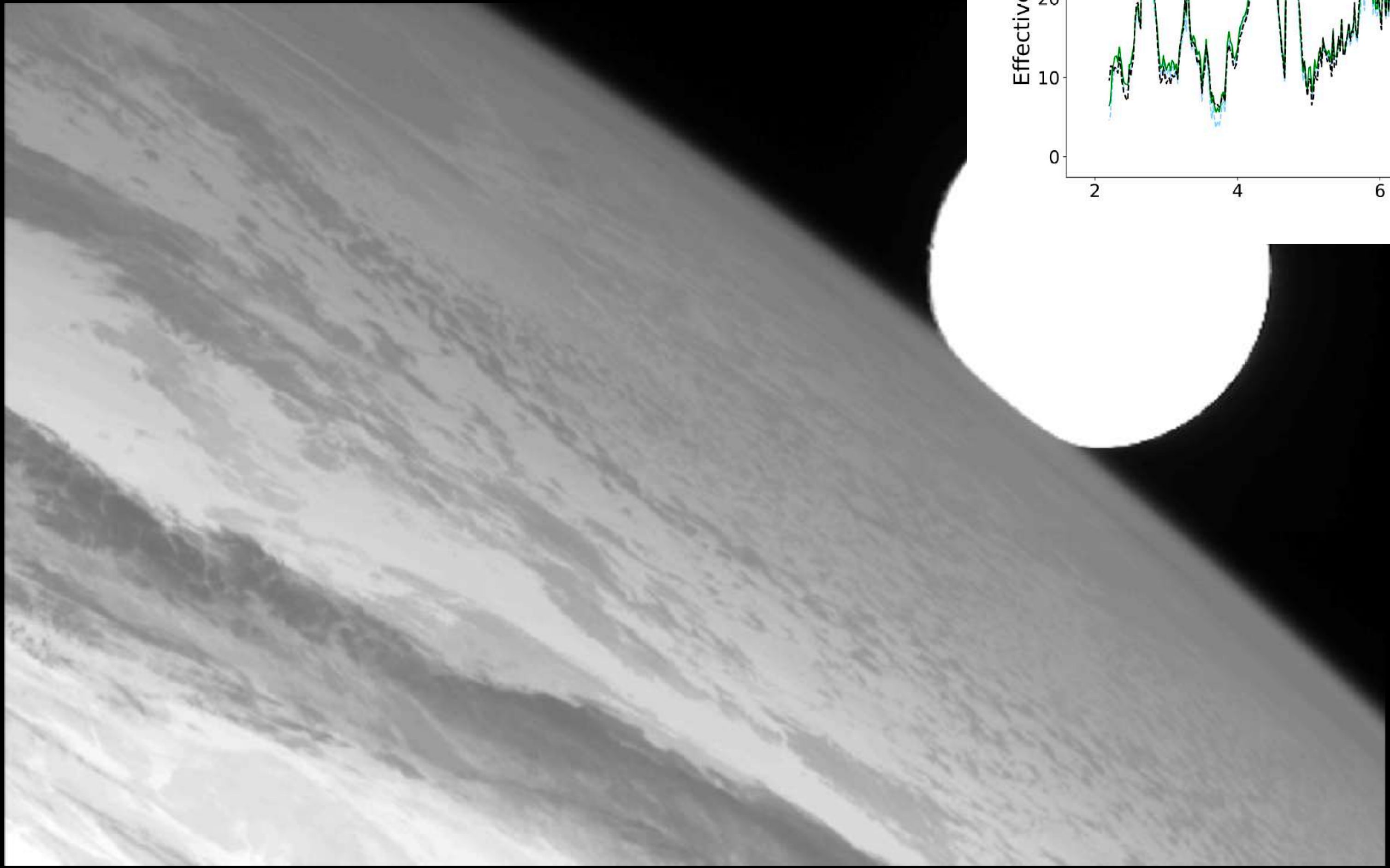
8.6 microns
spectral window (15 km)

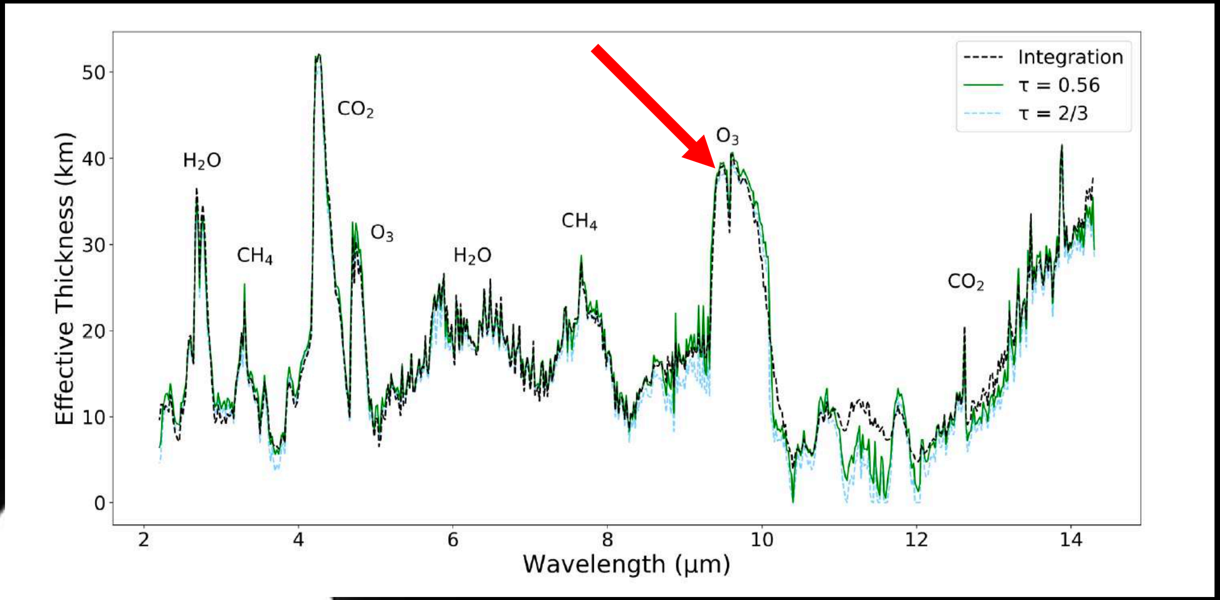




Credit: Himawary/Simon Proud/Vivien Parmentier

9.6 microns
O_3 band (40 km)





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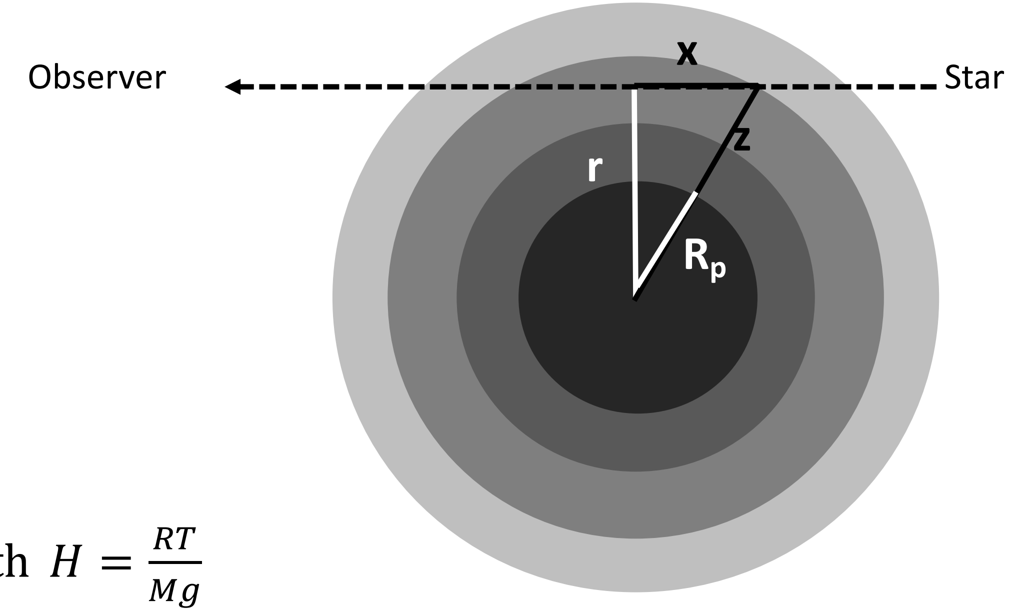
1D Forward models

Radiative transfer: transit spectroscopy



Ideal case:

- hydrostatic+isothermal
- cross-sections independent of P & T
- constant abundances

$$\tau(b,\lambda) = \sum_i \int_{-\infty}^{+\infty} \sigma_i(\lambda) n_i(x) dx \;;\; p(z) = p(z_0)\exp\left(-\frac{z-z_0}{H}\right) \text{ with } H = \frac{RT}{Mg}$$

$$n_i(x) = ni_0 e^{-z/H} \text{ with } z = \sqrt{r^2+x^2} - Rp \approx r - Rp + \frac{x^2}{2Rp}$$

$$\tau(r,\lambda) \approx \sum_i \sigma_i(\lambda) n_{i0} e^{-(r-Rp)/H} \int_{-\infty}^{+\infty} e^{-x^2/2RpH} dx = \sum_i \sigma_i(\lambda) n_{i0} e^{-(r-Rp)/H} H \sqrt{\frac{2\pi Rp}{H}}$$

Comparison with vertical optical depth:

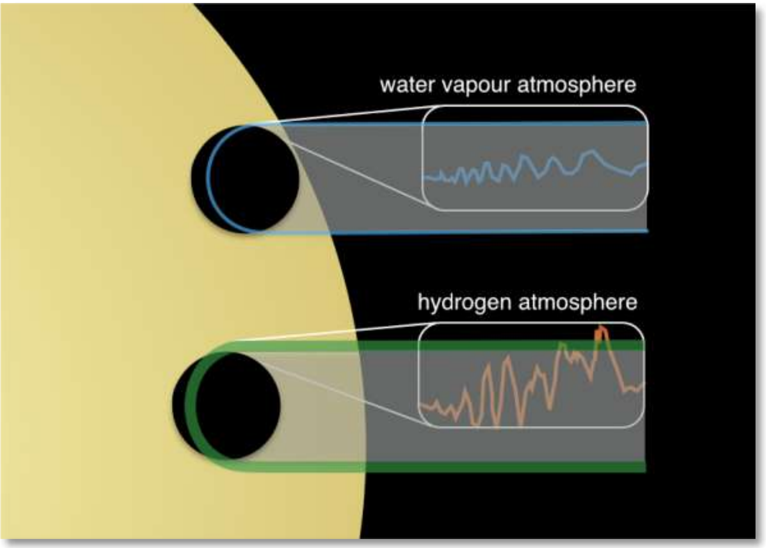
$$\boxed{\boldsymbol{\eta = \frac{\tau_H}{\tau_V} = \sqrt{\frac{2\pi Rp}{H}}}}$$

Earth: $\eta \sim 75$
K2-18 b: $\eta \sim 60$
HD209458 b: $\eta \sim 38$

Transits probe pressures 1-2 orders of magnitude lower than eclipses

1D Forward models

Radiative transfer: transit spectroscopy



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Variation of transit depth:

$\tau_1(r_1,\lambda_1) = \tau_2(r_2,\lambda_2) \approx 0.56$; $\boldsymbol{\Delta r = H ln\left(\frac{\sigma(\lambda_1)}{\sigma(\lambda_2)}\right)}$; $\boldsymbol{\Delta D = \frac{2RpHln\left(\frac{\sigma(\lambda_1)}{\sigma(\lambda_2)}\right)}{R_\star{}^2}}$

→ Transit spectroscopy easier for high scale height (e.g. hot giant planets)

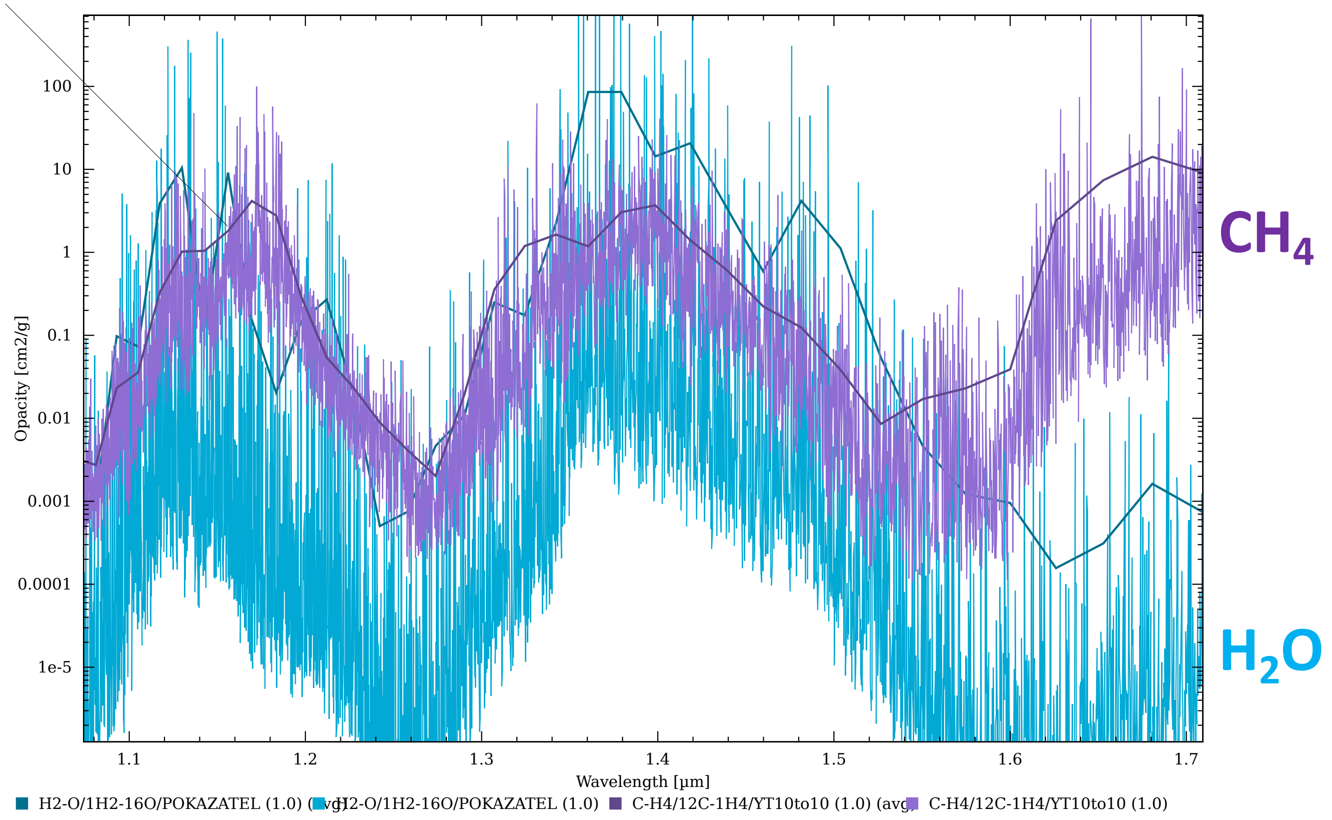
$$\frac{\sigma(\lambda_{max})}{\sigma(\lambda_{min})} \approx 10^3 \rightarrow \boldsymbol{\Delta r \approx 7H}$$

→ Transit depth at low resolution depends on the **mean value of $\boldsymbol{ln(\sigma)}$**

1D Forward models

Radiative transfer: transit spectroscopy

Opacity of H_2O and CH_4 (at 300K & 1 mbar) computed with the online tool DACE/OPACITY (https://dace.unige.ch/opacity/)



at 1.4 μm: $\frac{\overline{\sigma_{H_2O}}}{\overline{\sigma_{CH_4}}} \approx 10$; $\frac{\overline{\ln(\sigma_{H_2O})}}{\overline{\ln(\sigma_{CH_4})}} \approx 0.1$

H_2O should be masked by CH_4 at low resolution but not at high resolution

1D Forward models

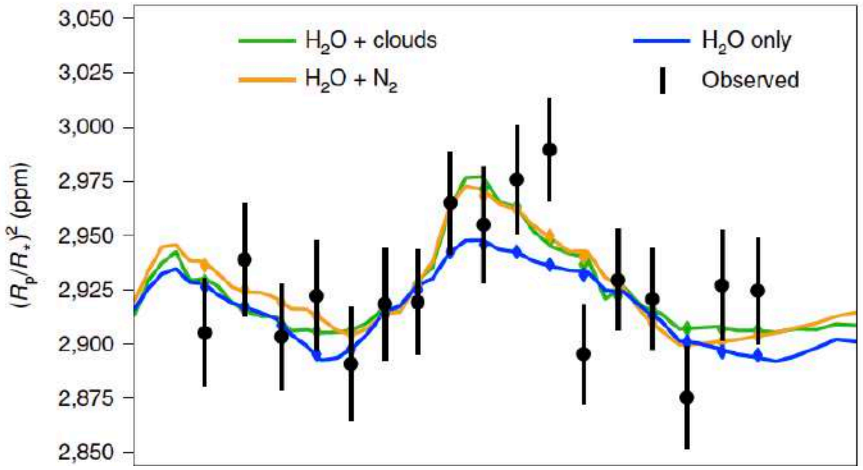
Radiative transfer: transit spectroscopy

Example K2-18 b:

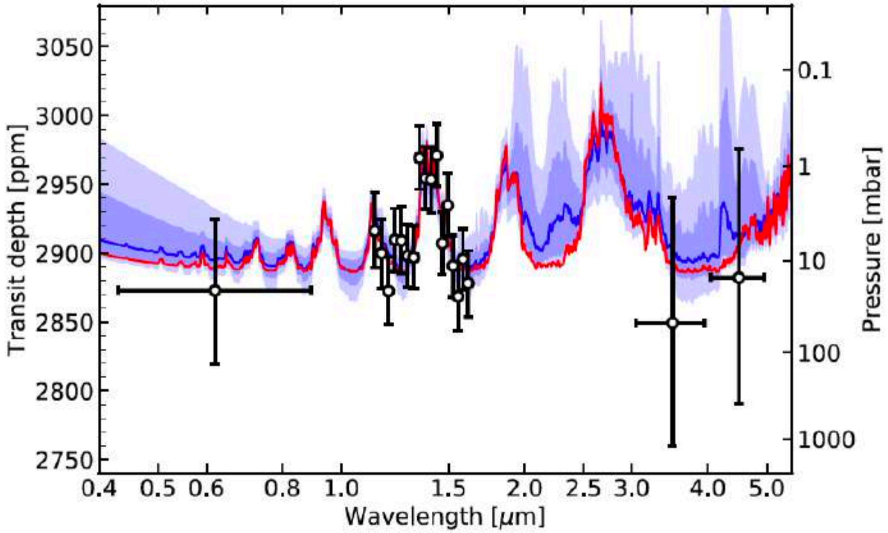
K2-18b:
Mass = 8.63 $M_\oplus$
Radius = 2.6 $R_\oplus$
Irradiation = 1368 W/m^2
(1361 W/m^2 for the Earth)
Orbital period = 33 days

A temperate sub-Neptune, with water vapour and potentially water clouds

HST transit spectrum



Tsiaras et al. (2019)



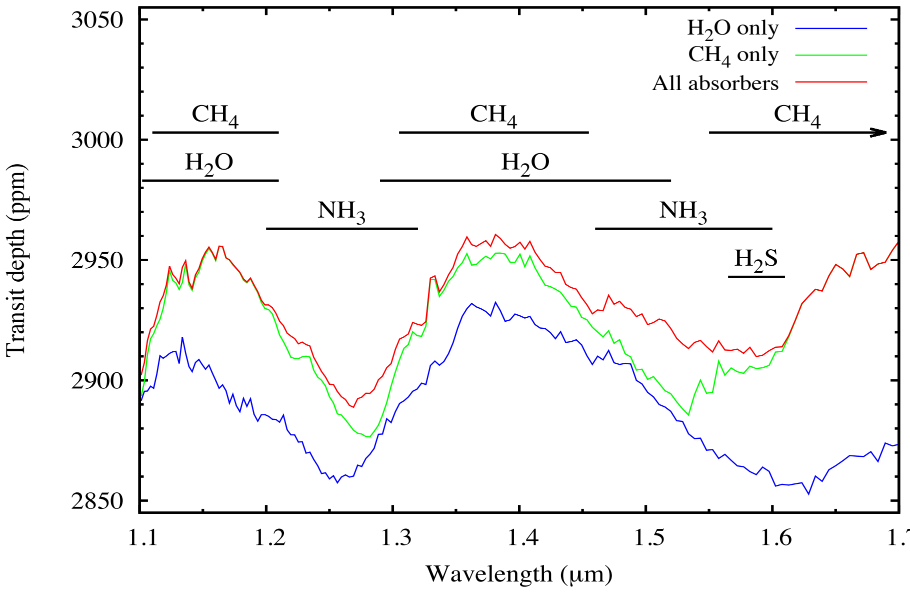
Benneke et al. (2019)

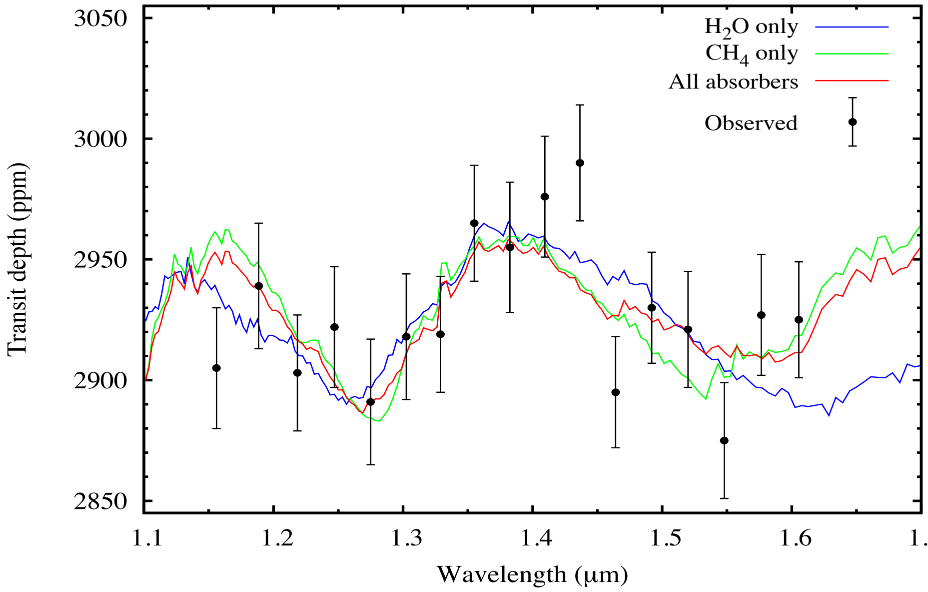
1D Forward models

Radiative transfer: transit spectroscopy

<u>Example K2-18 b:</u>

Transit spectra of K2-18 b computed with Exo-REM (metallicity=200×solar)





Bézard, Charnay & Blain (2022)

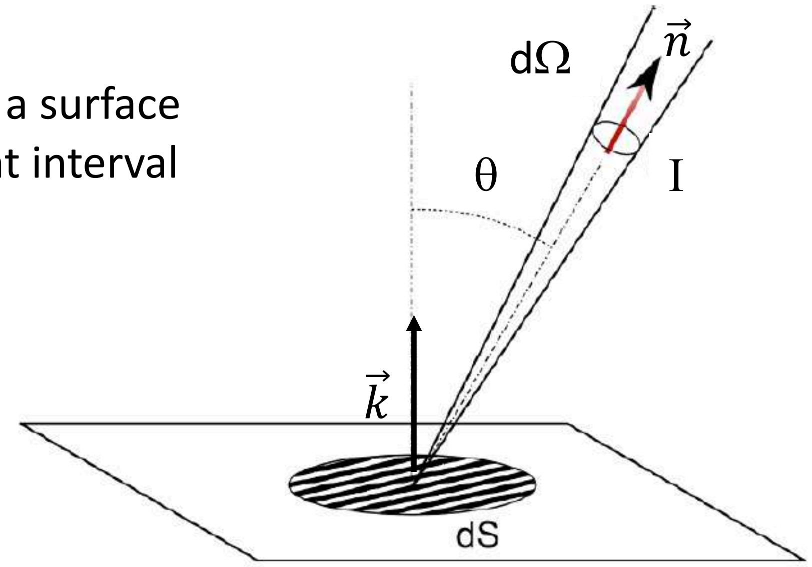
CH_4 should be the dominant absorber for a solar C/O
H_2O should be the dominant absorber for $C/O < 0.1 \times C/O_{solar}$

1D Forward models

Radiative transfer: definition of intensity and flux

Intensity $\boldsymbol{I}$ = amount of energy passing through a surface area dS, within a solid angle $d\Omega$, per wavelenght interval $d\lambda$, per unit time (I in J m^{-2} sr^{-1} μm^{-1}):

$$dE = I(x, \vec{n}, \lambda, t)\, \vec{n} \,.\, \vec{k}\; d\Omega\, dS\, d\lambda dt$$



Moments:

Mean intensity:
$$J = \int_\Omega I(x, \vec{n}, \lambda, t) d\Omega$$

Flux:
$$F = \int_\Omega I(x, \vec{n}, \lambda, t) \vec{n} \,.\, \vec{k} d\Omega = \iint I(x, \theta, \varphi, \lambda, t) cos(\theta) \sin(\theta)\, d\theta d\phi$$

1D Forward models

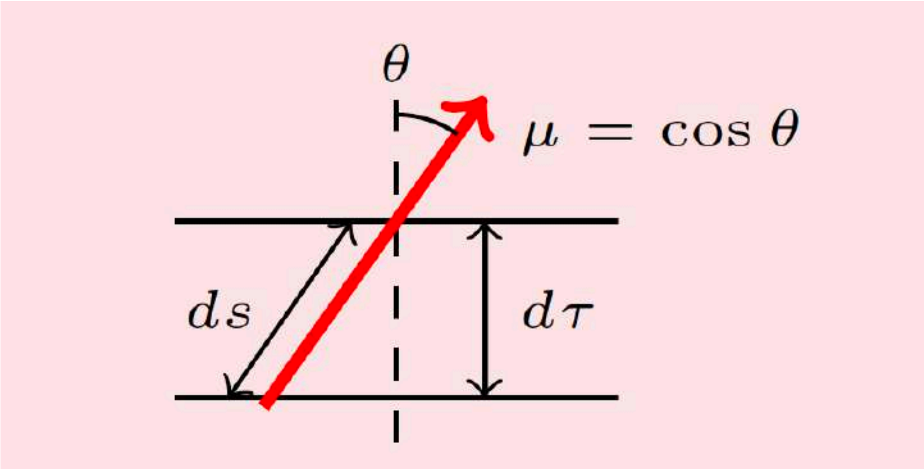
Radiative transfer: equation for plane-parallel

Optical depth & extinction coefficient:

$$d\tau = -k\,(T, P, \lambda)\;\mu\; ds$$

$$k(T, P, \lambda) = \sum_i n_i\,(\sigma_i{}^{abs} + \sigma_i{}^{scat})$$

Optical mean free path: $l = \frac{1}{k}$



Radiative transfer equation:

$$\boxed{\mu\,\frac{dI}{d\tau} = I - S}$$

Local thermodynamic Equilibrium (LTE):

$T_{radiation}$=$T_{kinetics}$

mean free path of photons ≪ length scale of T variations

1D Forward models

Solution a purely emitting atmosphere

$$\boxed{\mu \frac{dI}{d\tau} = I - B}$$

$$\boxed{B(T,\lambda) = \frac{2hc^2}{\lambda^5}\frac{1}{e^{hc/\lambda kT} - 1}}$$

Intensity at top of the atmosphere:

$$I(\tau = 0, \mu, \phi, \lambda) = B(T(\tau_0), \lambda)e^{-\frac{\tau_0}{\mu}} + \int_0^{\tau_0} B(T(\tau), \lambda)\; e^{-\tau/\mu}\frac{d\tau}{\mu}$$

Transmittance

Flux at top of the atmosphere (outgoing radiation):

$$F^{\uparrow}(\tau = 0, \lambda) = \int_0^{2\pi}\int_0^1 \mu I(\tau = 0, \mu, \phi, \lambda)\, d\mu d\phi$$

Resolution with Gauss-quadrature:

$$F^{\uparrow}(\tau = 0, \lambda) = 2\pi \sum_i^{N_g} \mu_i I(\tau = 0, \mu_i, \lambda)\, \omega_i$$

1D Forward models

The two-stream approximation

$$\boxed{\mu \frac{dI}{d\tau} = I - S}$$

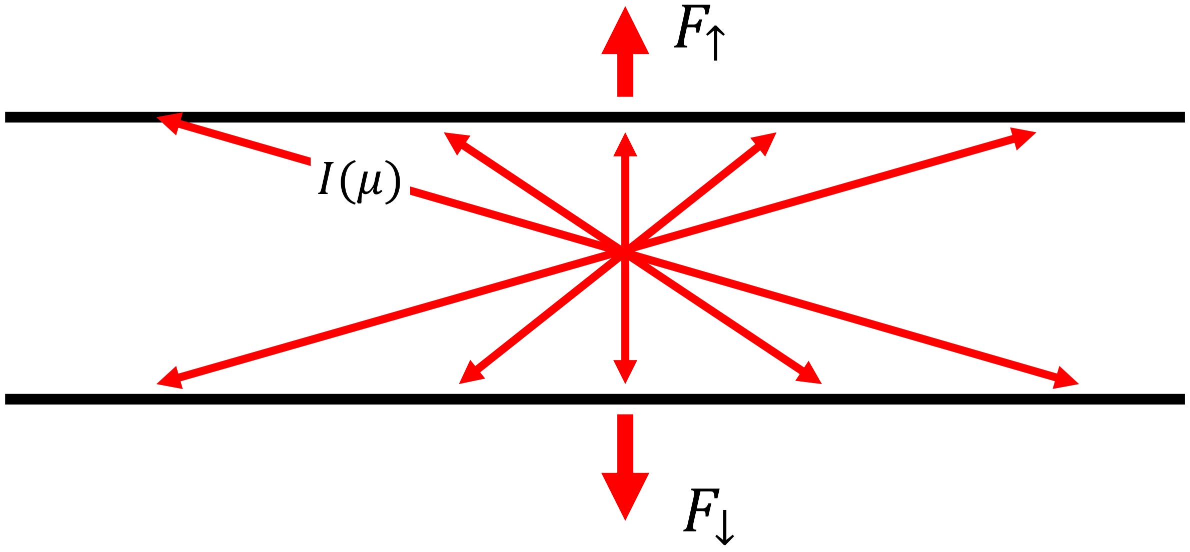
Goal: to compute the total upward and downward flux

$$J_\uparrow \equiv \int_0^{2\pi} \int_0^1 I \, d\mu \, d\phi,$$

$$J_\downarrow \equiv \int_0^{2\pi} \int_{-1}^0 I \, d\mu \, d\phi,$$

$$F_\uparrow \equiv \int_0^{2\pi} \int_0^1 \mu I \, d\mu \, d\phi,$$

$$F_\downarrow \equiv \int_0^{2\pi} \int_{-1}^0 \mu I \, d\mu \, d\phi,$$



The two-stream solution consists in approximating I so that it is related to F.

We assume $\frac{F^\uparrow}{J^\uparrow} = \frac{F^\downarrow}{J^\downarrow} = \frac{1}{\gamma} \Leftrightarrow \mu = \frac{1}{\gamma}$

(generally $\gamma = \sqrt{3}$)

1D Forward models

The two-stream approximation

Case of a purely emitting atmosphere:

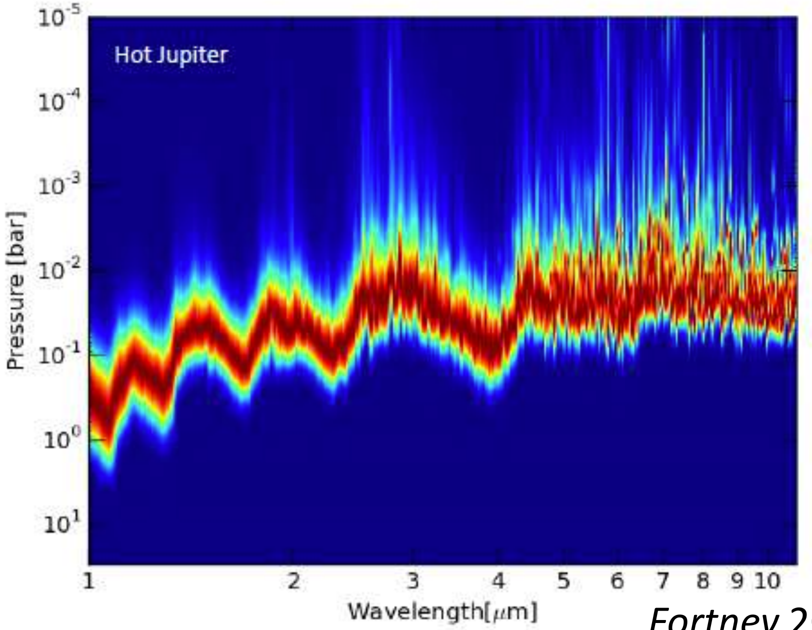
Outgoing radiation:

$$F^{\uparrow}(\tau = 0) = F^{\uparrow}(\tau_0)e^{-\gamma\tau_0} + \int_0^{\tau_0} 2\pi\gamma B e^{-\gamma\tau}\, d\tau$$

Transmittance

Weighting function:

$$cf(P) = B(\lambda, T)\frac{de^{-\gamma\tau}}{dlog(P)}$$



Fortney 2018

Peak of contribution:
at $\boldsymbol{\tau}$ **~2/3** also called the **photosphere**

Brightness temperature:
$\mathbf{T_b \sim T(\boldsymbol{\tau} = 2/3)}$

1D Forward models

Link between thermal structure and emission

Case of a purely emitting atmosphere:

Variation of thermal flux: $$\boxed{\frac{\delta F}{F} \approx -\frac{T}{B}\frac{\partial B}{\partial T}\frac{\mathbf{dlnT}}{\mathbf{dlnP}}\frac{\delta k}{k}}$$

For $\delta k > 0$:

- $\frac{\delta F}{F} < 0 \rightarrow \frac{dT}{dz} < 0$ (no thermal inversion)
- $\frac{\delta F}{F} > 0 \rightarrow \frac{dT}{dz} > 0$ (thermal inversion)
- $\frac{\delta F}{F} \approx 0 \rightarrow \frac{dT}{dz} \approx 0$ (isothermal)

The emission spectrum with/without thermal inversion

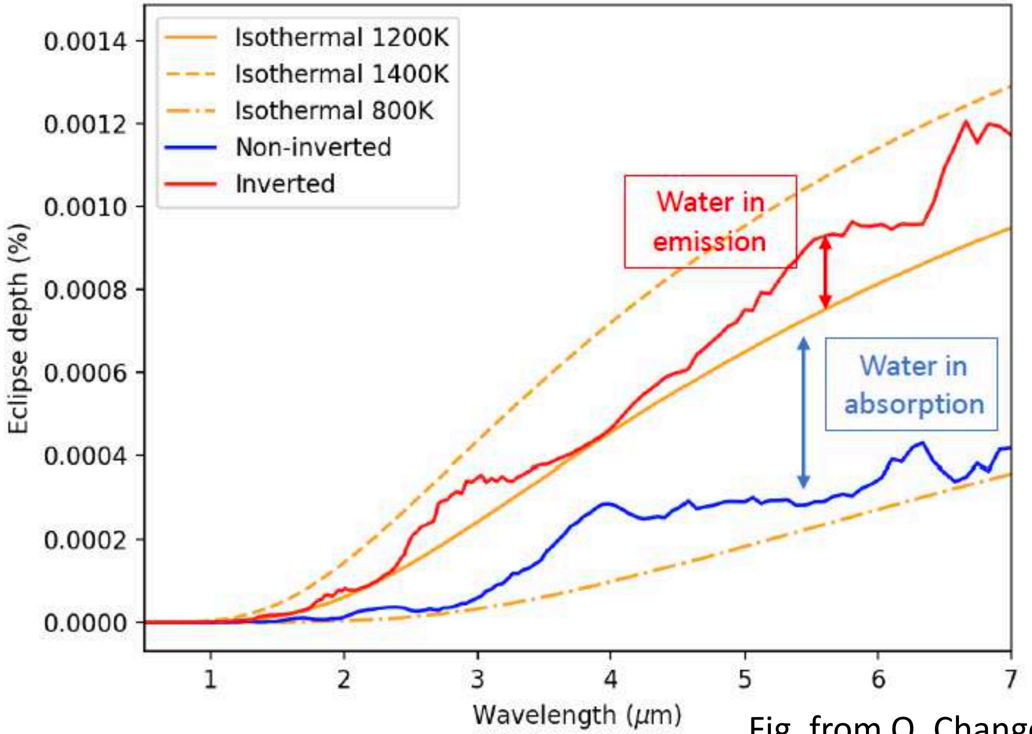
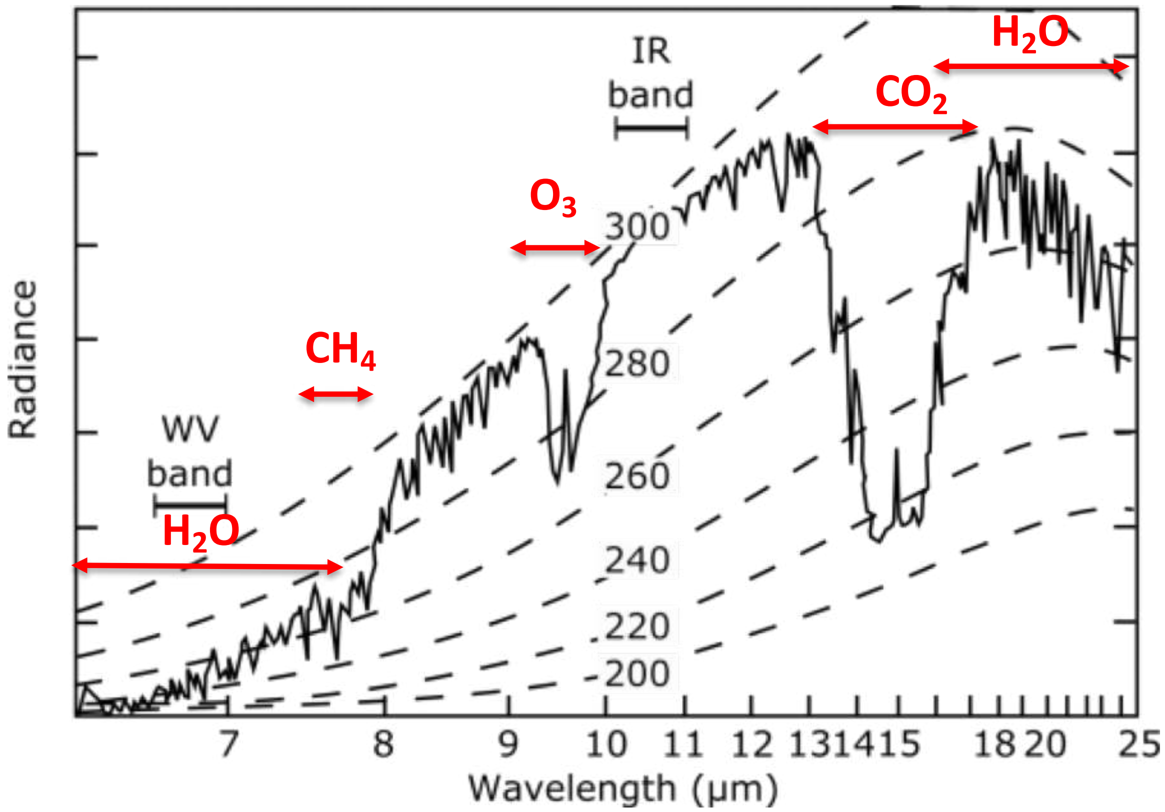


Fig. from Q. Changeat

1D Forward models

Link between thermal structure and emission

Earth's thermal emission

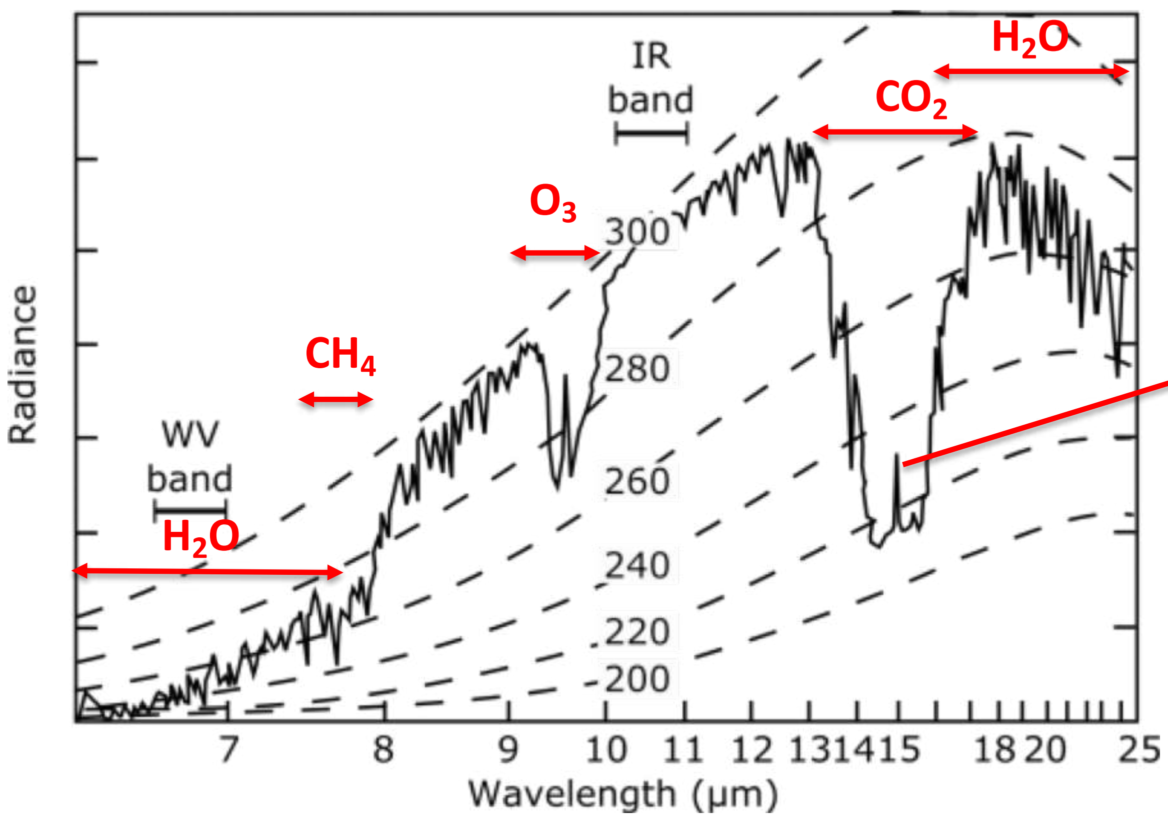


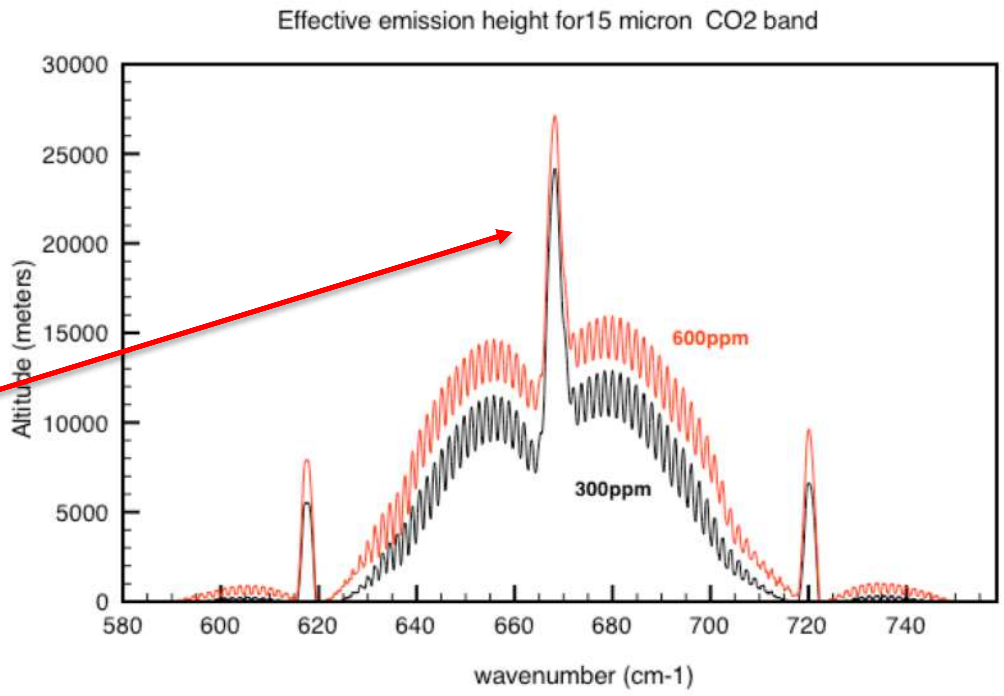
Where is the signature of the stratospheric thermal inversion in the emission spectrum ?

1D Forward models

Link between thermal structure and emission

Earth's thermal emission





1D Forward models

Methods for solving RT

General case of the two-stream approximation
(thermal emission + scattering)

$$\frac{\partial F^{\uparrow}}{\partial \tau} = \gamma_1 F^{\uparrow} - \gamma_2 F^{\downarrow} - 2\pi(1-\omega_0)B$$
$$\frac{\partial F^{\downarrow}}{\partial \tau} = \gamma_2 F^{\uparrow} - \gamma_1 F^{\downarrow} + 2\pi(1-\omega_0)B$$

Method	γ_1	γ_2	μ_*
Quadrature	$\sqrt{3}[1-\omega_0(1+g)/2]$	$\sqrt{3}\omega_0(1+g)/2$	$1/\sqrt{3}$
Hemispheric mean	$2-\omega_0(1+g)$	$\omega_0(1-g)$	$1/2$

Quadrature for deep atmosphere & Hemispheric mean for the upper atmosphere

See *Toon et al.* (1989) for the complete solution with multi-layers

1D Forward models

Methods for solving RT

1) <u>Semi-grey analytical model</u>

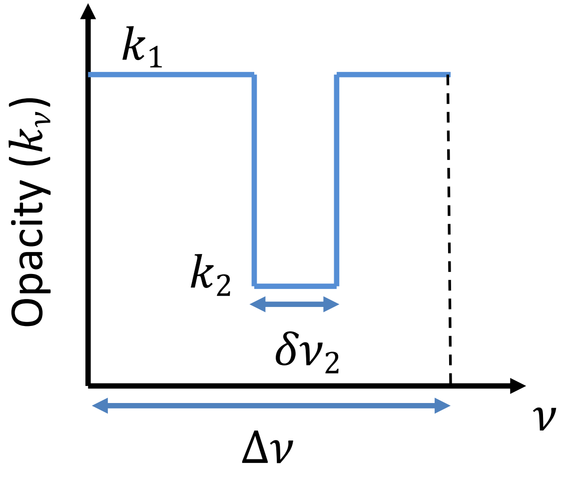
➡ Only for computing the thermal structure (e.g. for retrieval or thermal evolution)

- <u>Model of *Guillot et al.* (2010):</u>

  Two parameters (k_{vis} and k_{ir}) for visible (stellar) and infrared (planetary) radiation

- <u>Models with sub-bands:</u>
  e.g. *Parmentier et al.* (2014) and *Robinson & Catling* (2012):

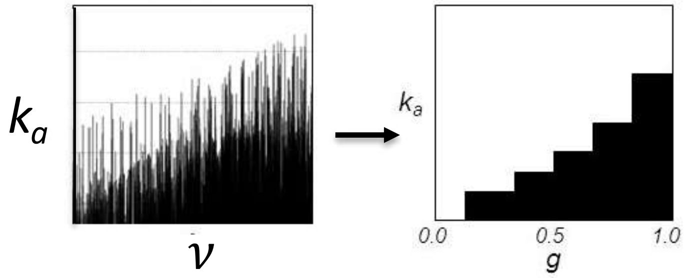
  One parameter for visible (k_{vis}) and three parameters for infrared (k_{ir1}, k_{ir2}, $\beta = \frac{\delta\nu_2}{\Delta\nu}$)



2) <u>Correlated-k method</u>

Multiple sub-bands representative f the distribution of opacity inside a large band

➡ **Fast method, excellent for low and medium resolution**
Can combine different molecular species
Widely used for atmospheric models and 3D GCM



1D Forward models

Methods for solving RT

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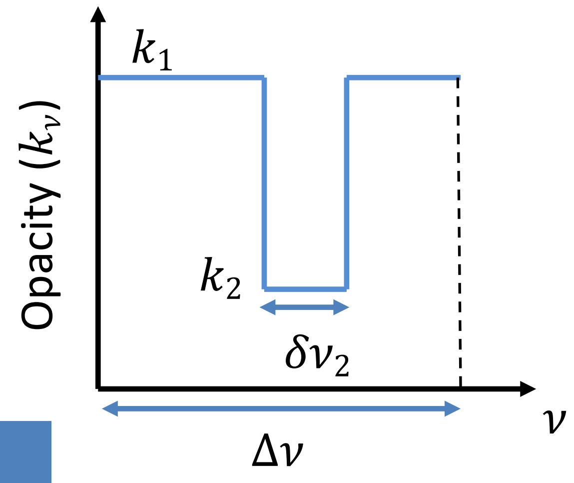


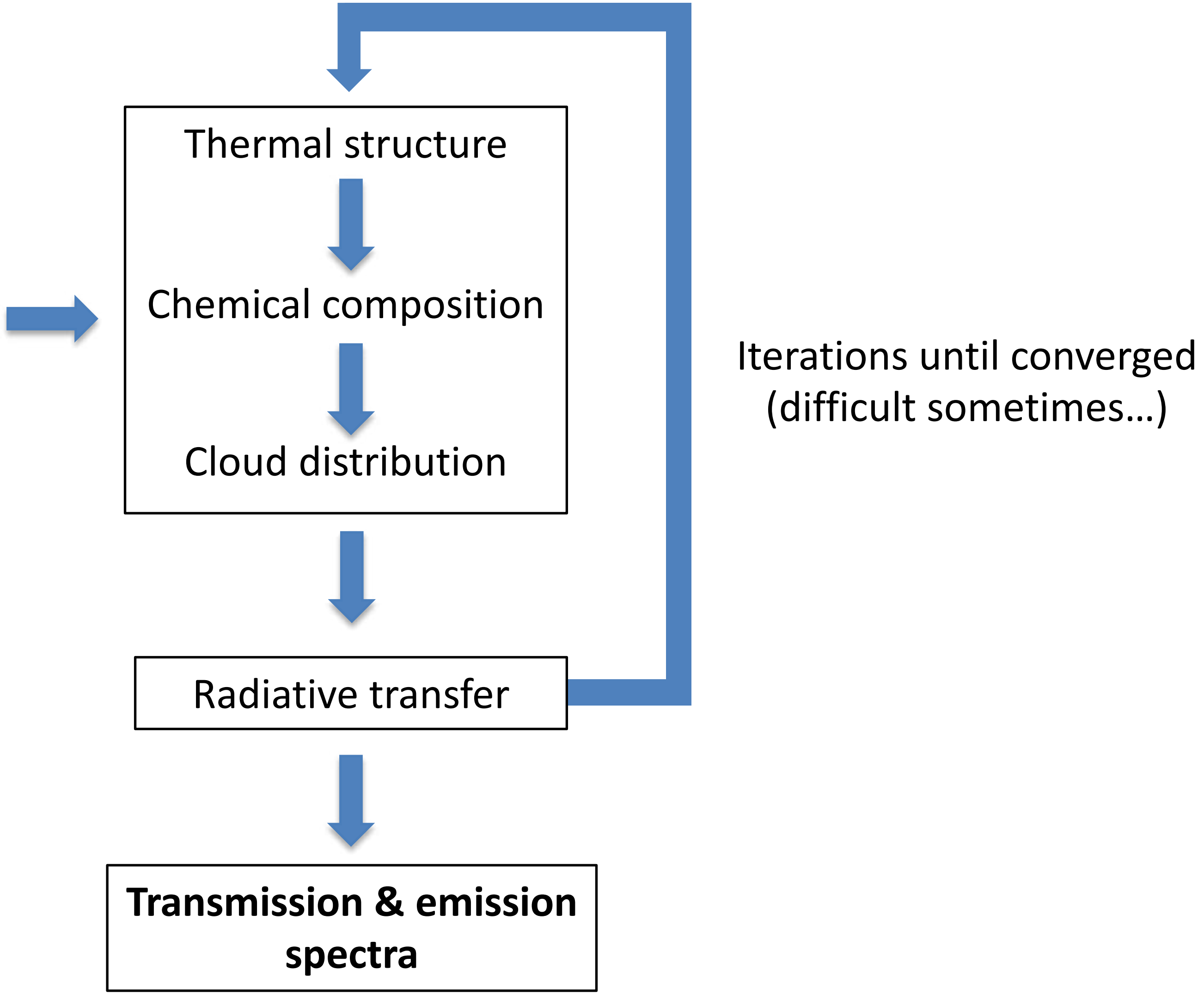
2) <u>Correlated-k method</u>

Exo_k: tool to compute kcoefficients for different formats
(PCM GCM, Exomol, Nemesis, PetitCode, TauREx, Exo-REM, ARCIS):
http://perso.astrophy.u-bordeaux.fr/~jleconte/exo_k-doc/index.html

1D Forward models

Self-consistent models

Input parameters:
- Planetary radius
- Gravity
- Irradiation
- T_{int}
- Metallicity
- C/H, O/H, N/H,…
- Initial TP profile
- Opacities



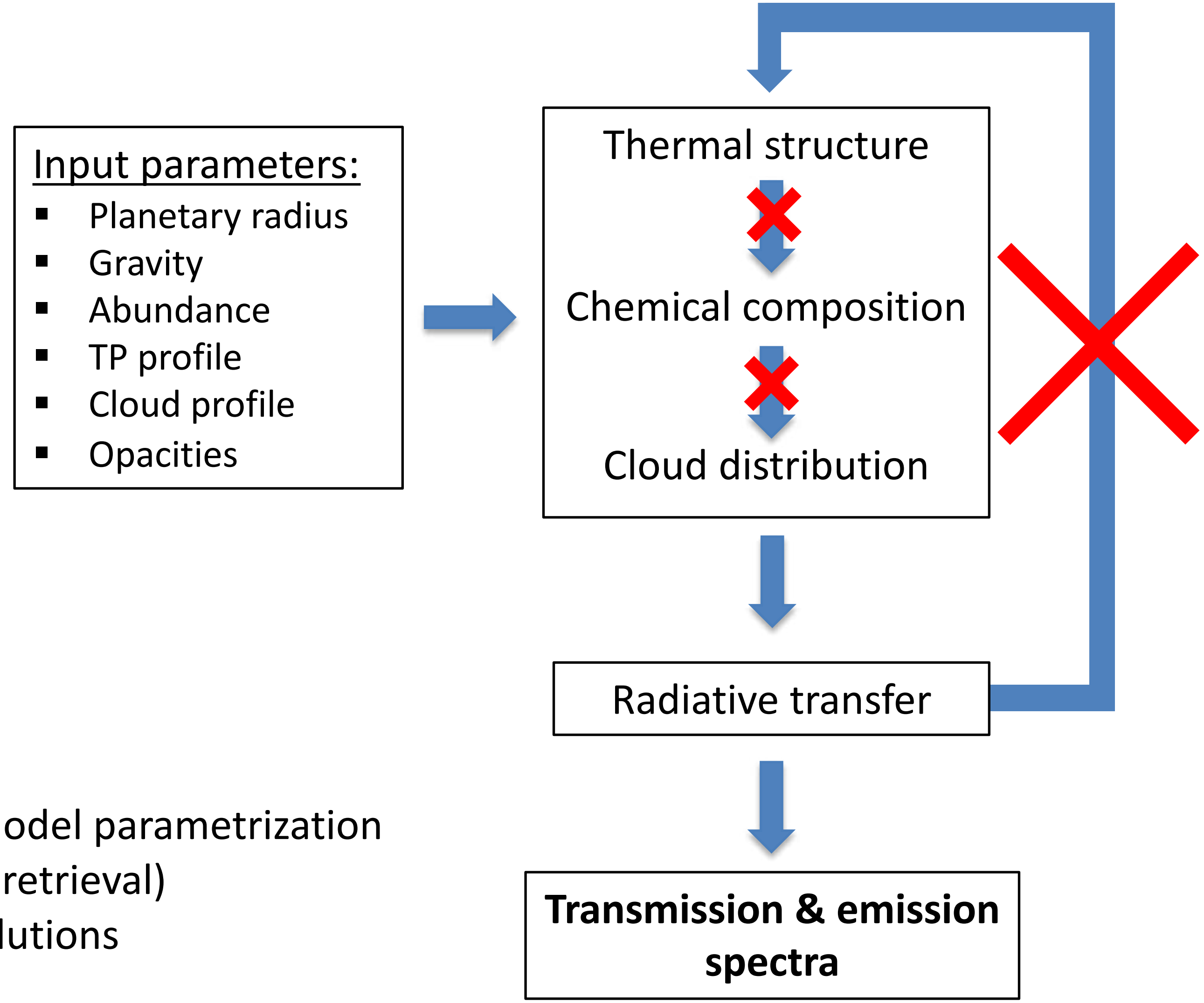
Models available online:
Exo-REM, PICASO, ATMO, PetitCode, Exo_k

Avantage/disavantages:
+ Physical solutions
- Solutions biased by model parametrization
- Slow (cannot be run online in retrieval)

→ Ideal for limited dataset or limited parameter exploration and for predicting/interpreting observations

1D Forward models

Parametric models



Avantage/disavantages:

+ Solutions not biased by model parametrization
+ Fast (can be run online in retrieval)
- Can provide unphysical solutions

→ Ideal for atmospheric retrieval without be biased by model parametrizations

Retrieval techniques

Chi2 with model grids

- ➢ Simplest method, used in particular for self-consistent models

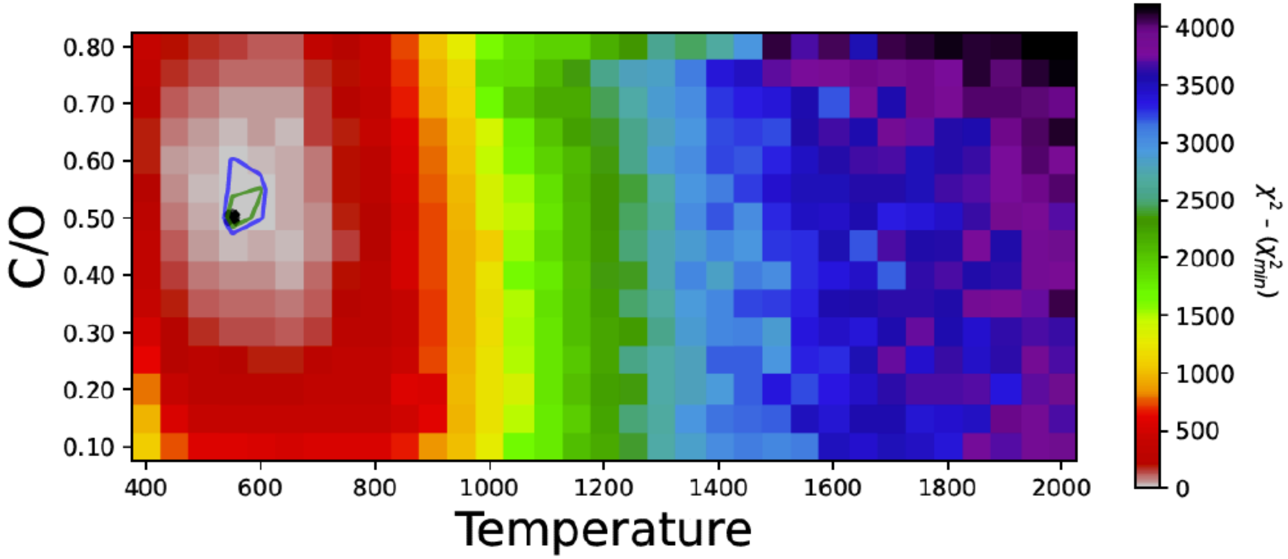
- ➢ Principe:
- N measurements $F_i^{obs} \pm \sigma_i$ (uncorrelated)
- F_i^{model} from a model
- Minimization of the cost function:

$$\boxed{\chi^2 = \sum_{i=1}^{n} \frac{\left(F_i^{obs} - F_i^{model}\right)^2}{{\sigma_i}^2}}$$

Simulation of GJ 504 b with MIRI-MRS (Mâlin et al. in prep):

- ➢ Contours of constant χ^2 :

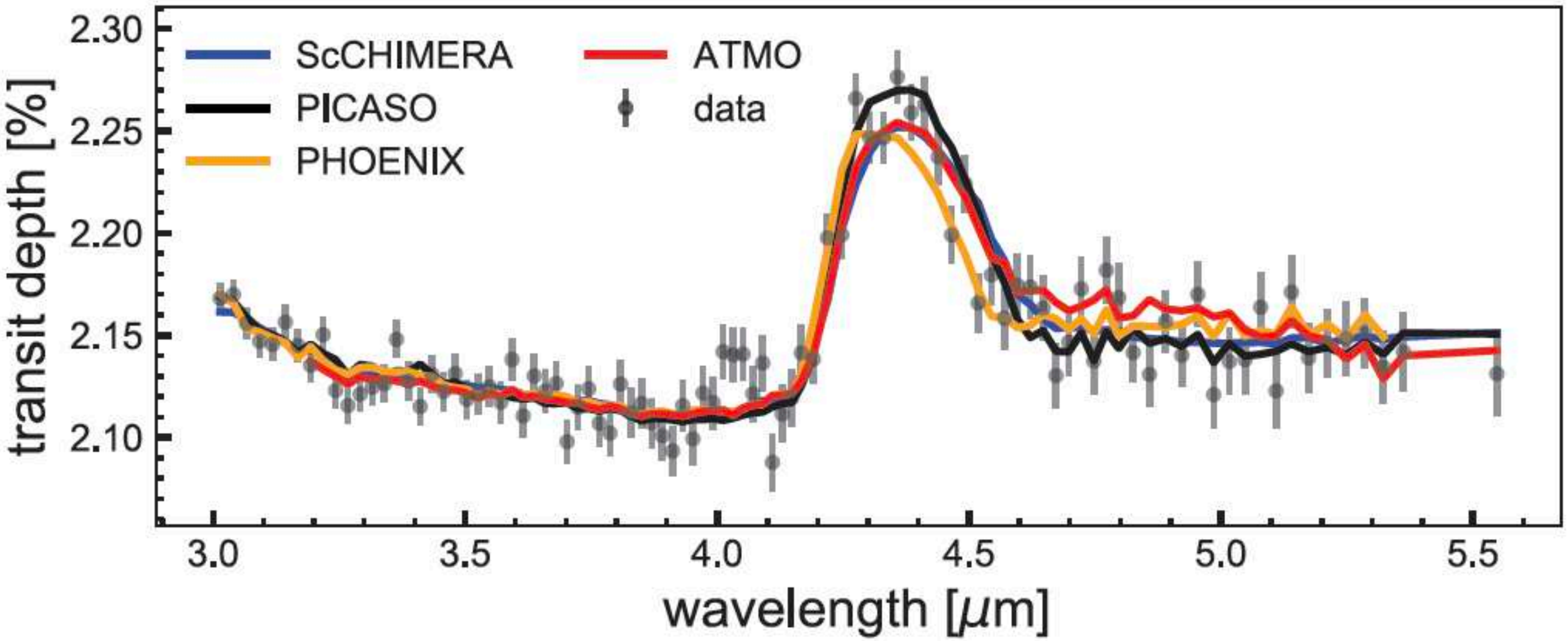
$$\chi^2 = \chi^2_{min} + \Delta\chi^2$$



Retrieval techniques

Chi2 with model grids

JWST-NIRSpec spectrum of WASP-39 b (ERS)



Retrieval techniques

Bayesian inference (MCMC & Nested-sampling)

A simple retrieval with a Guillot TP profile (5 parameters) + 3 molecule abundances (e.g. H_2O, CH_4, CO) + clouds (P_{top}) + Rp = 10 free parameters !

→ **A statistical method is required to explore the parameter space, focusing on the best fits**

➢ **Bayesian inference**

Likelihood function of the data

Prior probability of the model

Posterior probability of the model

$$P(\text{model}|\text{data}) = \frac{P(\text{data}|\text{model})\text{P}(\text{model})}{P(\text{data})}$$

Evidence [not important because absorbed into the normalisation of the posterior]

Retrieval techniques

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A simple retrieval with a Guillot TP profile (5 parameters) + 3 molecule abundances (e.g. H_2O, CH_4, CO) + clouds (P_{top}) + Rp = 10 free parameters !

→ A statistical method is required to explore the parameter space, focusing on the best fits

- **Bayesian inference**

$$P(\text{model}|\text{data}) \propto P(\text{data}|\text{model})P(\text{model}) \propto \exp(-\chi^2/2)$$

We assume the prior is constant

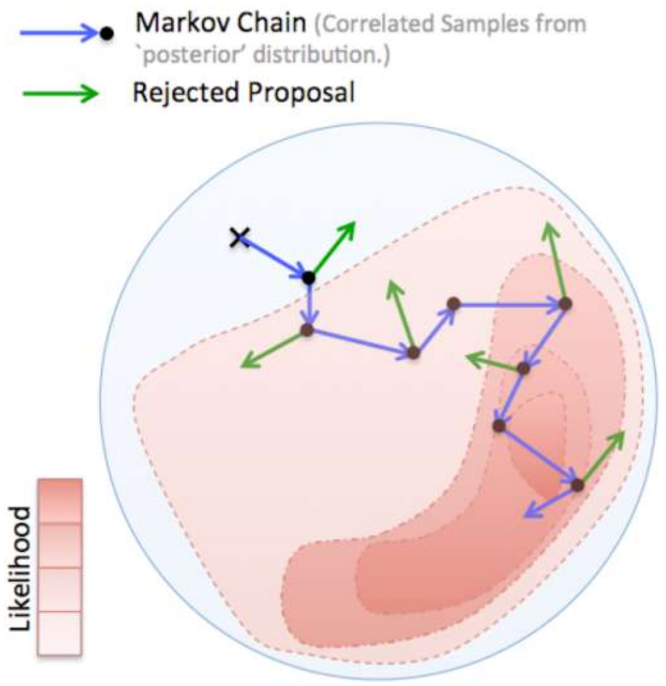
Likelihood function

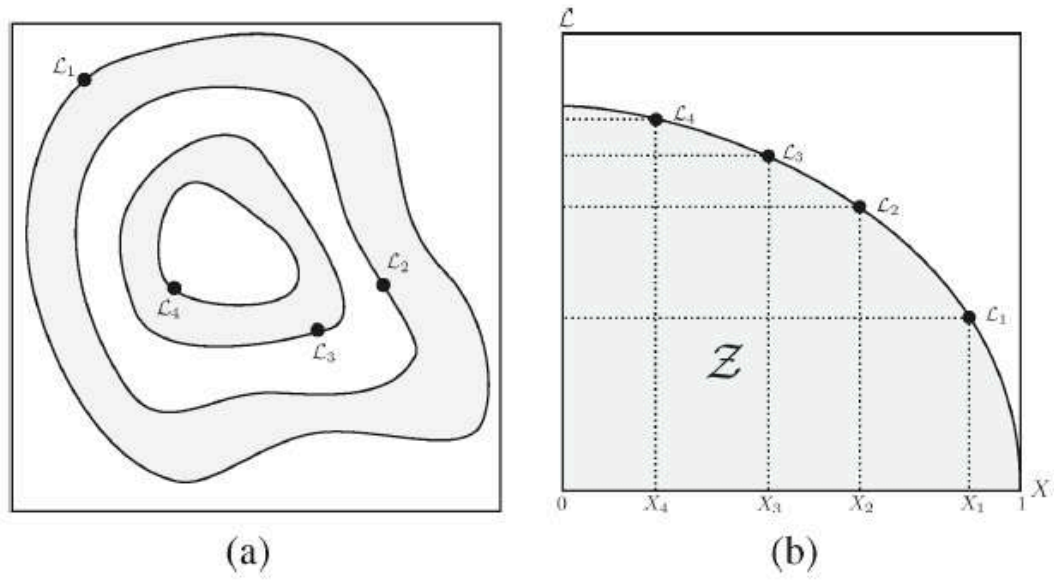
Retrieval techniques

Bayesian inference (MCMC & Nested-sampling)

1) Markov chain Monte Carlo (MCMC)

2) Nested Sampling





Ensemble of walkers converging toward best solutions
(e.g. Pyrat Bay, Madhusudhan et al.)

Determination of volumes of equal likelihood
(e.g. **Tau-Rex, petitRADTRANS,** NEMESIS, ARCiS, CHIMERA)

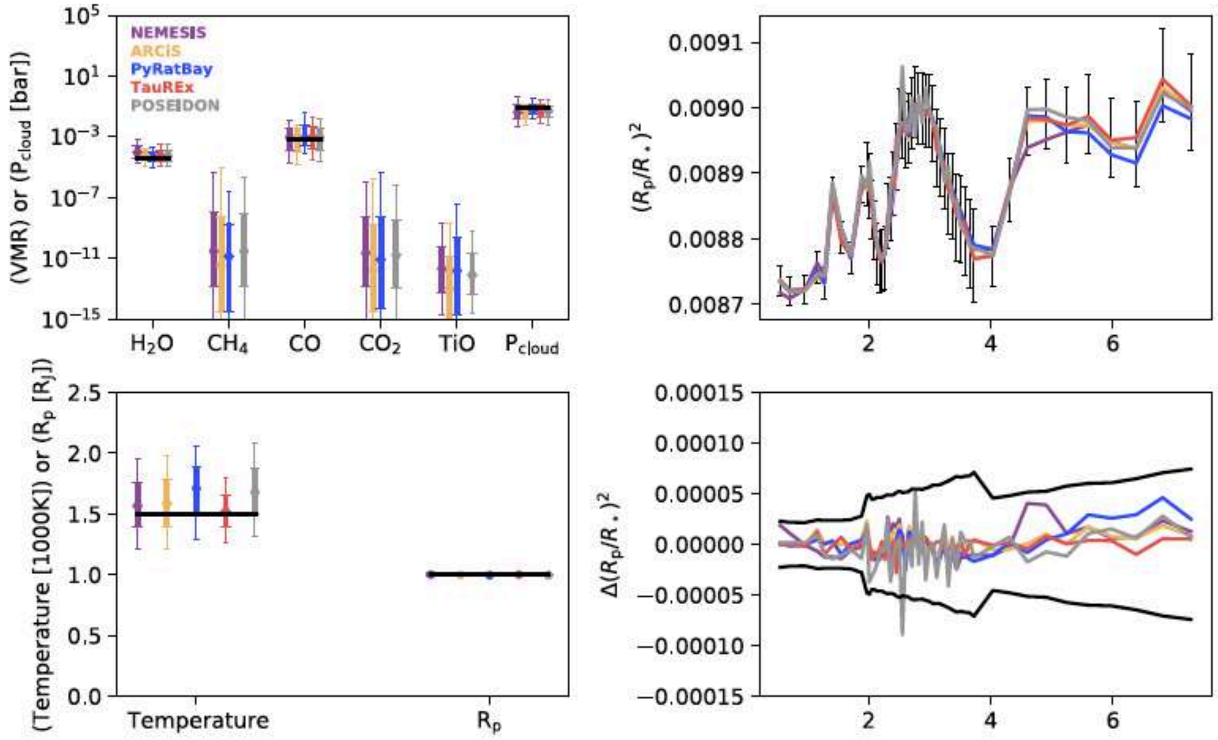
Nested sampling is more efficient to find global maximums of the likelihood

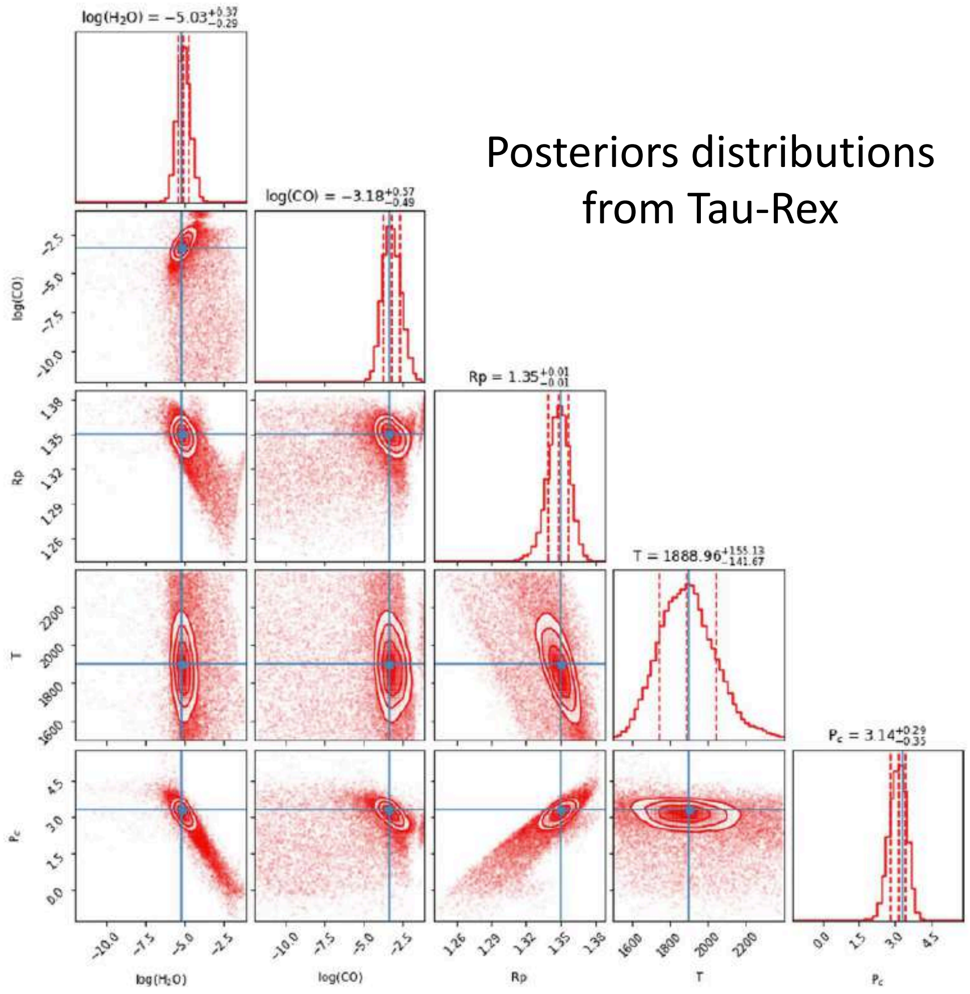
Retrieval techniques

Bayesian inference (MCMC & Nest-sampling)

Intercomparison of retrieval tools for Ariel (Barstow et al. 2022)

Cloudy warm Neptune





Posteriors distributions
from Tau-Rex

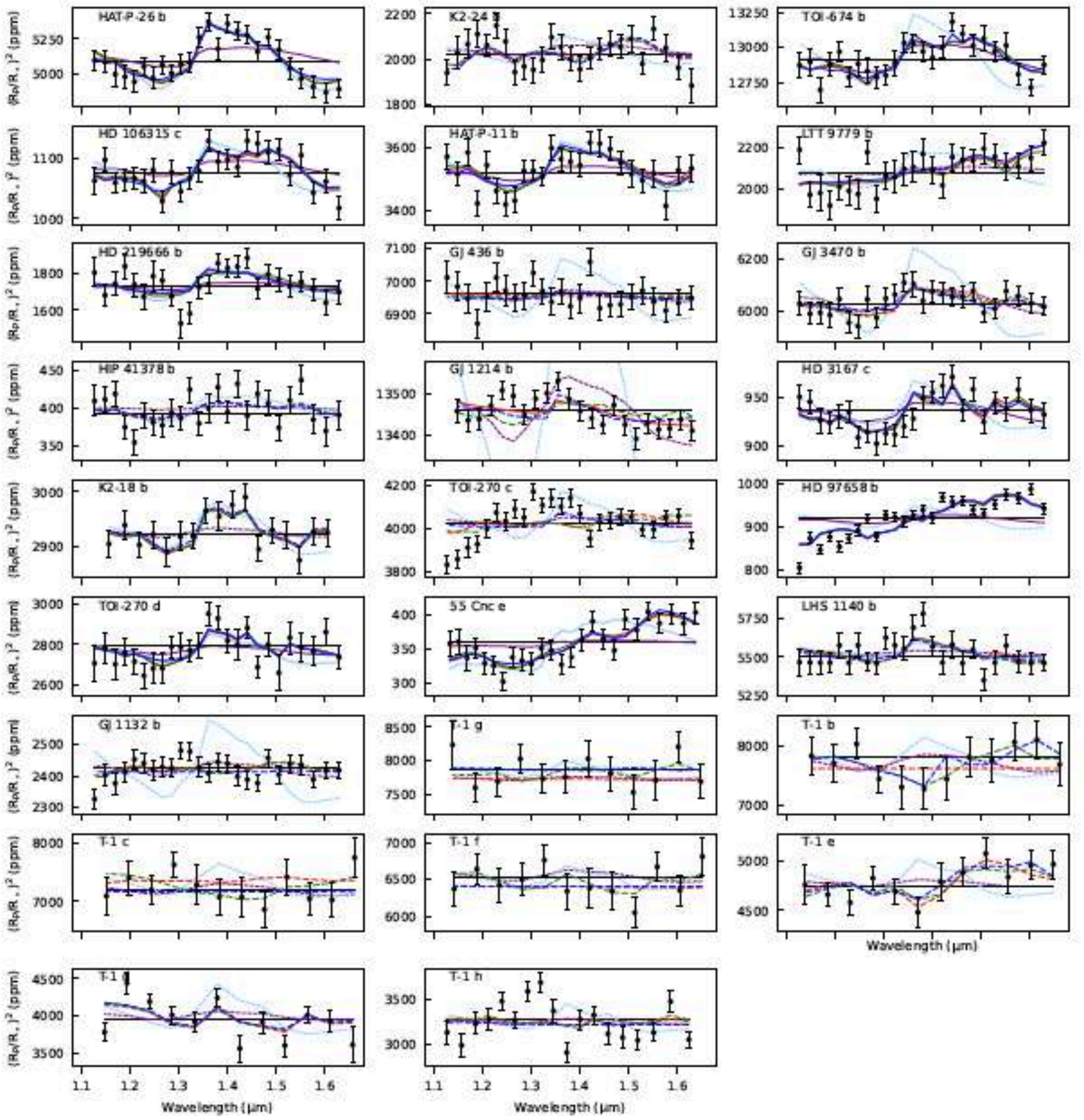
Barstow et al. 2022

Retrieval techniques

Bayesian inference (MCMC & Nest-sampling)

Strength of molecular detection with Bayes factor

Planet	Best-fit model	Δlog(E)	Detection	Absorbers (X)	μ (g/mol)
55 Cancri e	**2-Active clear**	29.94	strong	HCN	2.34
GJ 436 b	1-Primary	0.04	none	H_2O	2.31
GJ 1132 b	6-Flat-line	-	none	-	2.30
GJ 1214 b	**3-Hidden absorber**	3.53	strong	H_2O, N_2	27.90
GJ 3470 b	5- Water world	2.15	weak	H_2O	18.02
HAT-P-11 b	**2-Active clear**	9.99	strong	H_2O	4.43
HAT-P-26 b	**4-Primary clear**	43.12	strong	H_2O	2.32
HD 3167 c	**2-Active clear**	11.13	strong	H_2O, CO_2	2.84
HD 97658 b	**2-Active clear**	103.34	strong	HCN, CO_2[a]	2.85
HD 106315 c	**2-Active clear**	16.63	strong	H_2O, NH_3	5.94
HD 219666 b	**2-Active clear**	5.02	strong	H_2O	2.60
HIP 41378 b	4-Primary clear	2.44	weak	H_2O	2.32
K2-18 b	**2-Active clear**	3.47	strong	H_2O	2.43
K2-24 b	2-Active clear	0.39	none	NH_3	4.71
LHS 1140 b	**4-Primary clear**	3.70	strong	H_2O	2.32
LTT 9779 b	**2-Active clear**	5.71	strong	CO_2	2.31
TOI-270 c	2-Active clear	1.36	weak	CO_2	27.51
TOI-270 d	**2-Active clear**	5.19	strong	H_2O, CO_2	2.44
TOI-674 b	**5-Water world**	17.86	strong	H_2O[b]	8.87
TRAPPIST-1 b	2-Active clear	1.05	weak	CO, NH_3	2.39
TRAPPIST-1 c	6-Flat-line	-	none	-	2.30
TRAPPIST-1 d	3-Hidden absorber	0.59	none	H_2O	2.32
TRAPPIST-1 e	1-Primary	0.49	none	NH_3	2.32
TRAPPIST-1 f	1-Primary	0.10	none	-	2.31
TRAPPIST-1 g	6-Flat-line	-	none	-	2.30
TRAPPIST-1 h	6-Flat-line	-	none	-	2.30



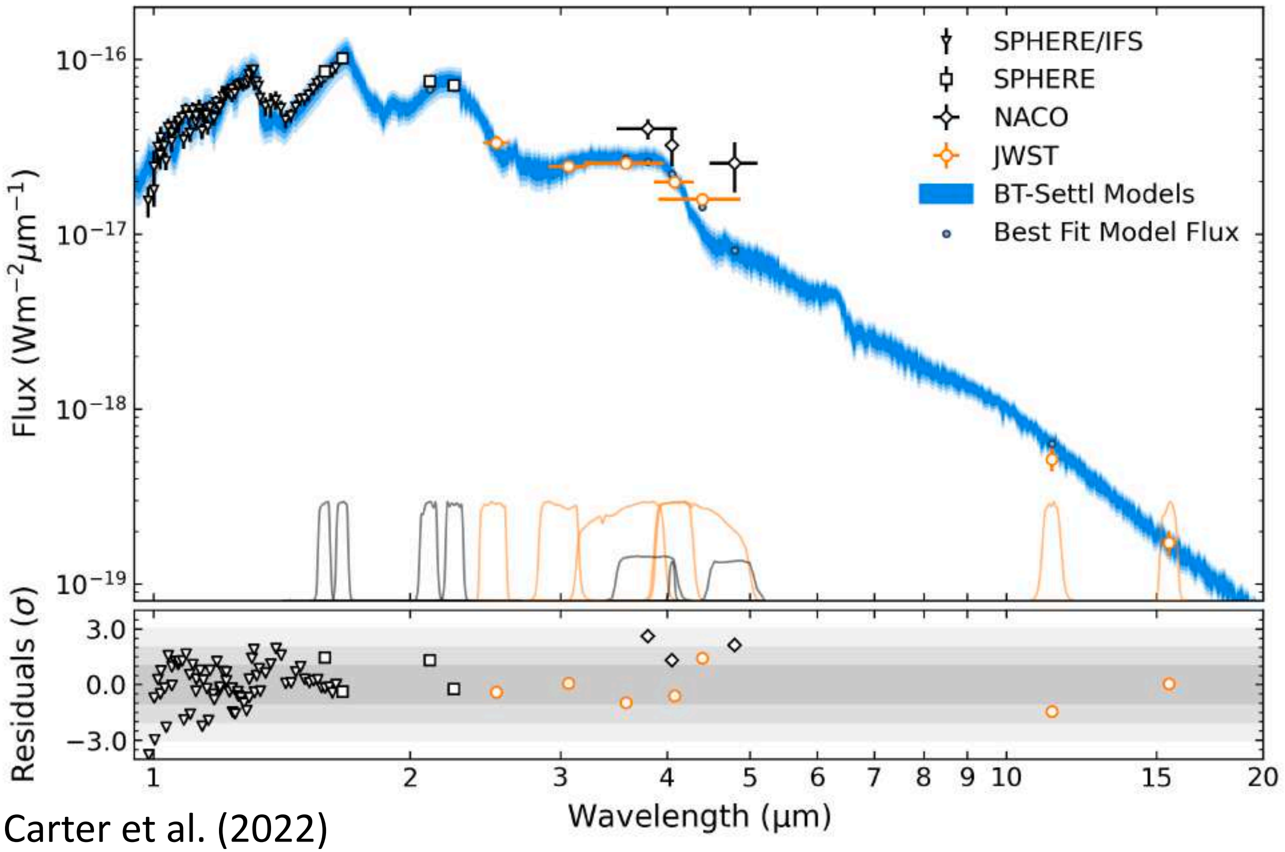
Gressier et al. (submitted)

Retrieval techniques

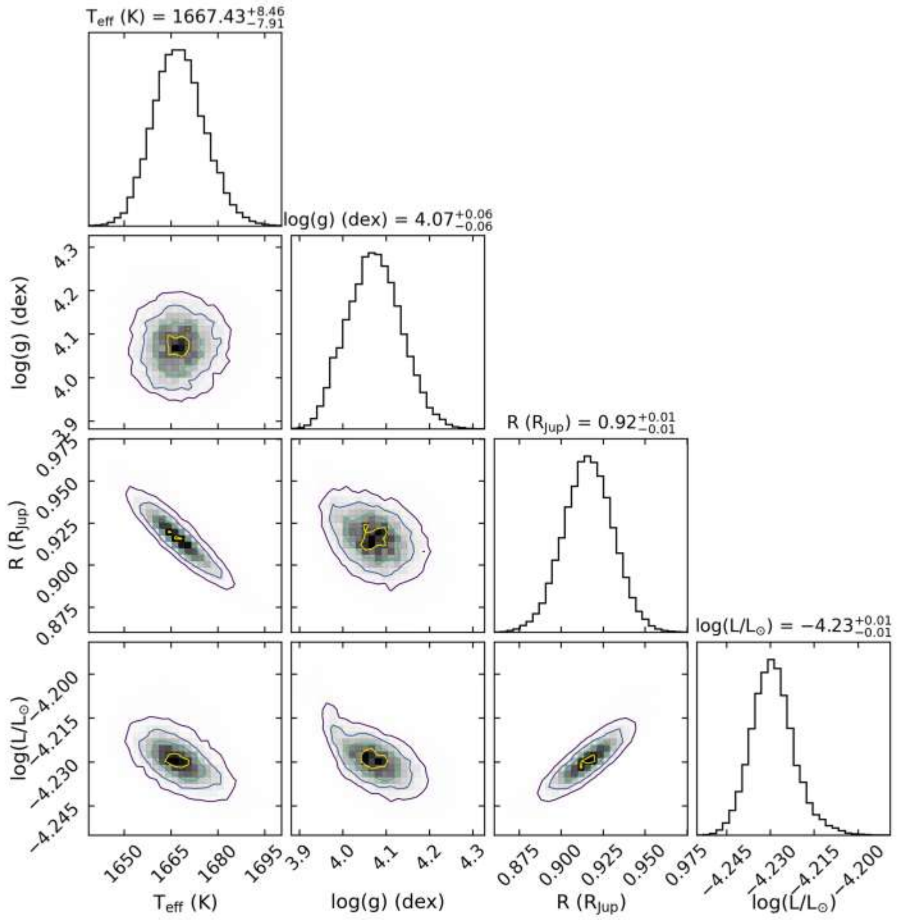
Bayesian inference (MCMC & Nest-sampling)

Interpolated model grid for MCMC

JWST imaging of HIP 65426 b from 2-16 micron



Carter et al. (2022)



Interesting for model grids with more than 3 parameters

Retrieval techniques

Optimisation estimation

Method widely used for Earth atmosphere remote sensing and for solar system atmospheres

<u>Principe:</u>

Minimization of a cost function:

$$J(x) = \underbrace{\big(y - F(x)\big)^T \underbrace{S_e^{-1}}_{\text{Error covariance matrix}} \big(y - F(x)\big)}_{\chi^2} + \underbrace{(x - x_a)^T \underbrace{S_a^{-1}}_{\text{A priori covariance matrix}} (x - x_a)}_{\text{Weight of the a priori + correlation between parameters}}$$

y = data vector
x = model parameter vector
x_a = a priori vector
$F(x)$ = forward model

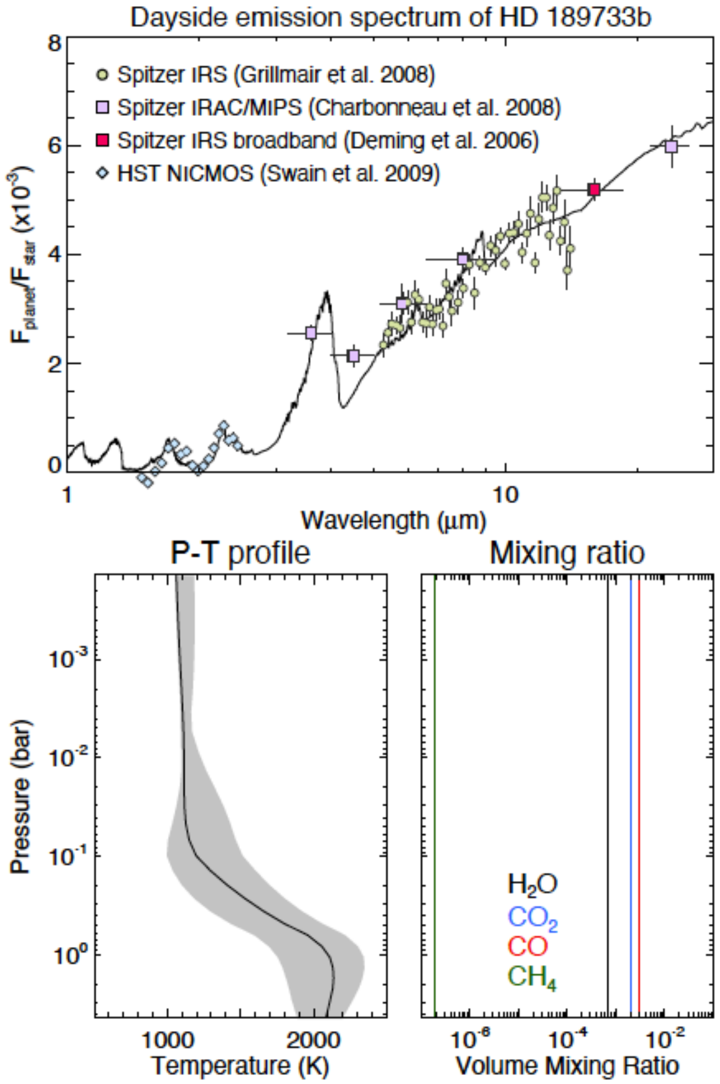
Correlation between temperatures of layer i and j: $S_{a,ij} = \left(S_{a,ii} S_{a,jj}\right)^{1/2} e^{\frac{-\left|\ln\left(\frac{P_i}{P_j}\right)\right|}{h}}$

Length of correlation

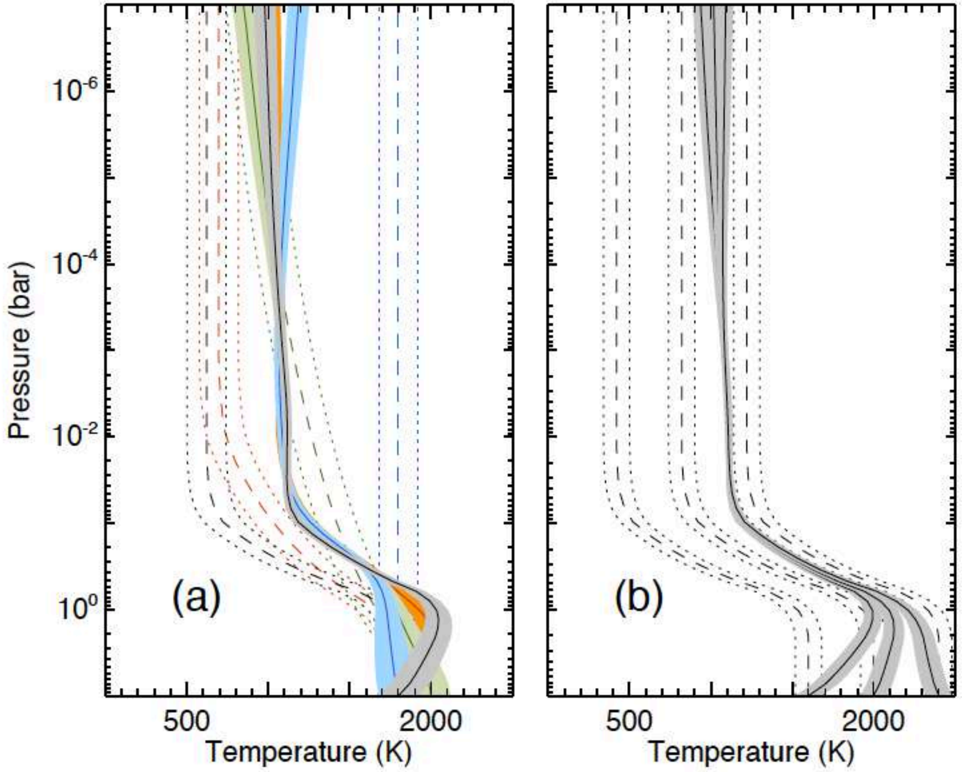
→ Algorithm to iterate toward a state minimizing J

Retrieval techniques

Optimisation estimation



Exploration of the impact of the a priori TP profile



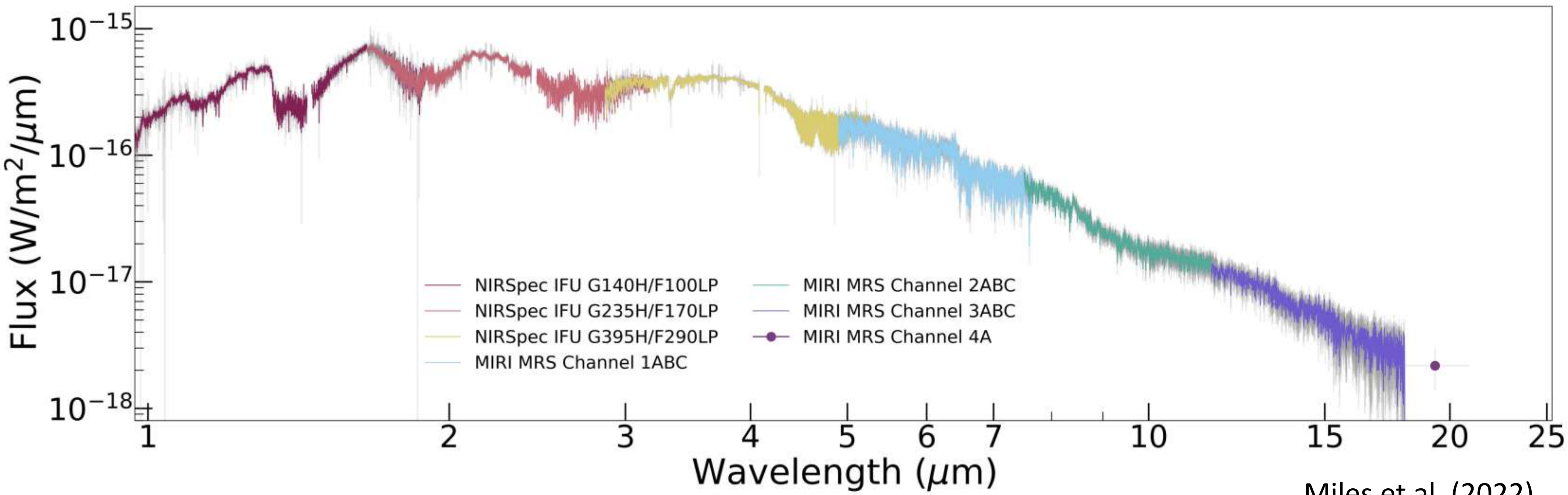
Lee et al. 2011
(NEMESIS)

- A priori profiles can be provided by self-consistent models but their impact must be analysed
- Optimisation estimation is a fast method, ideal for high quality data or with additionnal constraints

Retrieval techniques

Optimisation estimation

NIRSpec/MIRI-MRS spectrum of VHS 1256 b



Miles et al. (2022)

Optimisation estimation has a great potential for brown dwarfs and young giant planets

Avantages/disavantages of each method

Chi2 with model grids:
+ Computed just once
- Limited number of free parameters
- Strongly biased by model parametrizations

→ Ideal for limited parameter exploration (i.e. 2D/3D simulations) or low quality dataset

Bayesian inference (MCMC & Nested Sampling):
+ Better estimation of uncertainties than Chi2 maps and shows correlations
+ Exploration a large parameter space
+ Model selection (Bayes factor)
- Not efficient for retrieving profiles

→ Ideal for most cases for exoplanets

Optimisation estimation:
+ Efficient for retrieving profiles
+ Faster than Bayesian inference
- Requires a priori
- Limited exploration of possible solutions

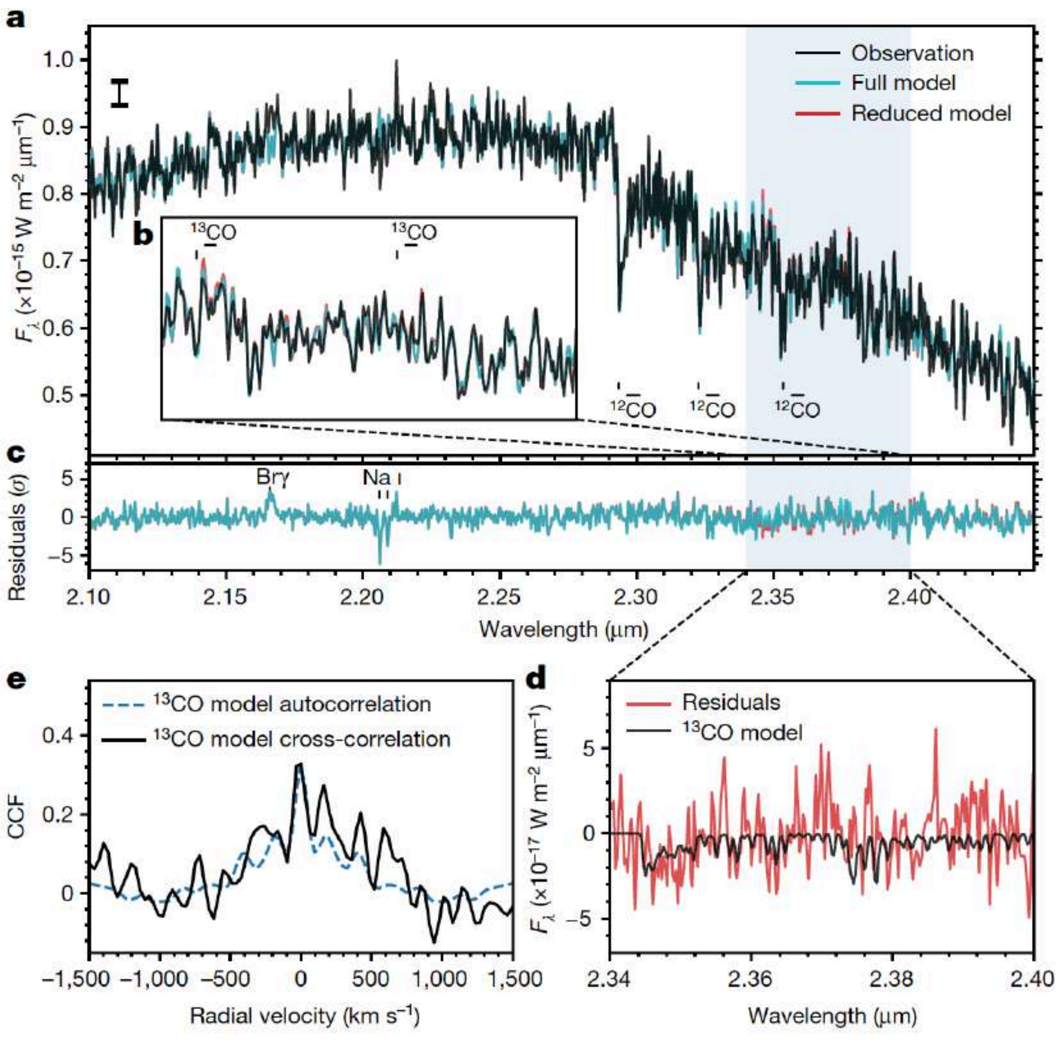
→ Ideal for emission spectroscopy with high-quality dataset and additional constraints

A combinaison of methods/models can be very useful

Lessons from models and retrieval

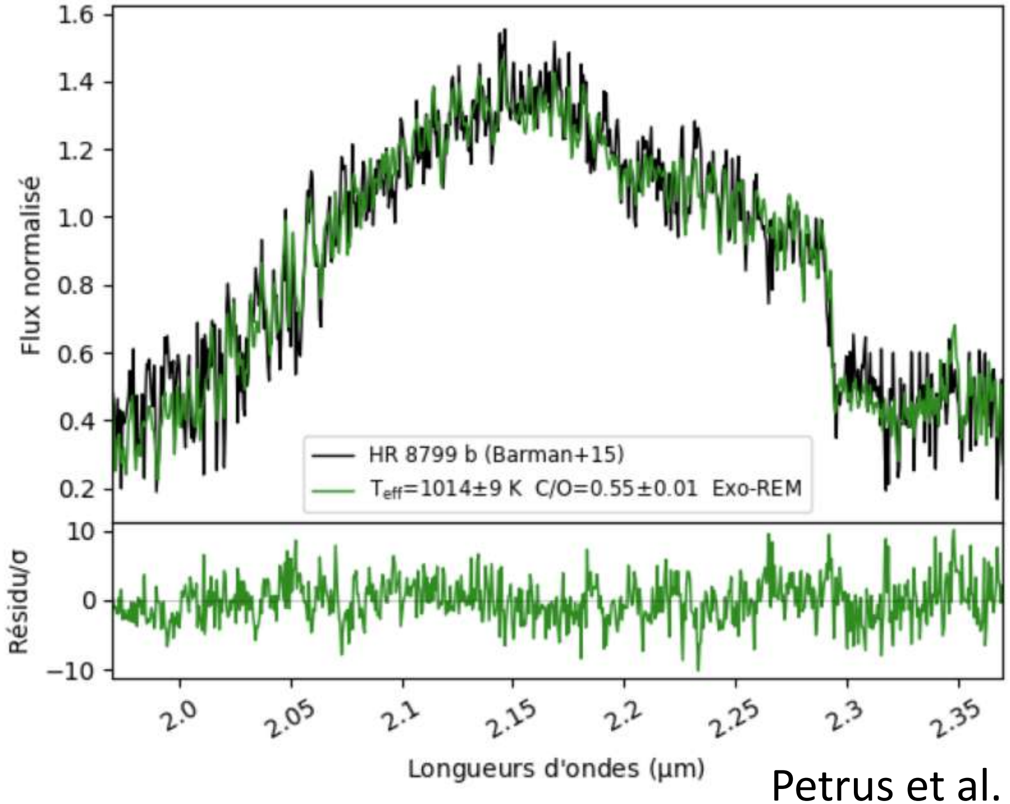
1) Atmospheric models work !

TYC 8998-760-1 b



Zhang et al. (2022)

HR8799 b



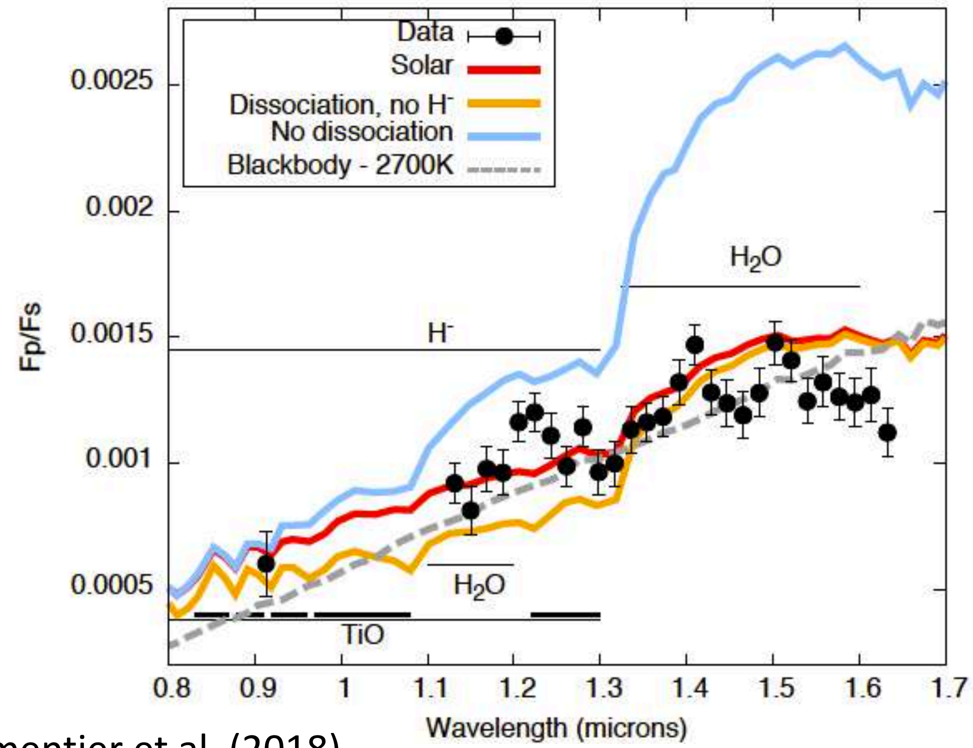
Petrus et al. *in prep*

Lessons from models and retrieval

1) Atmospheric models work !

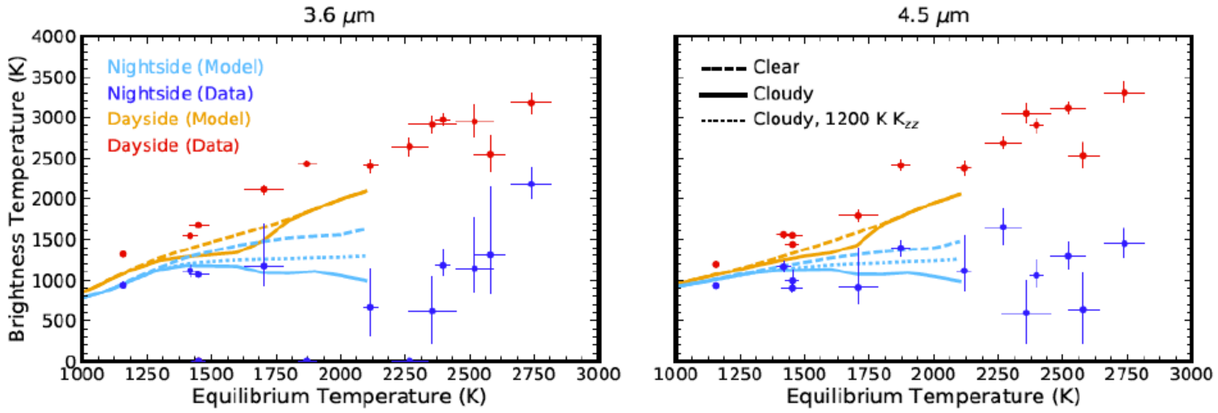
Two main reasons for cases for which models do not work: missing physical processes or 3D effects

Exemple #1: H^- in ultra-hot Jupiters

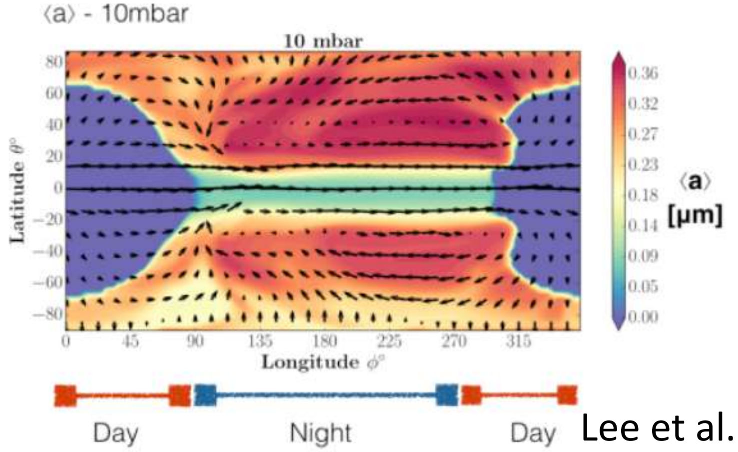


Parmentier et al. (2018)

Exemple #2: nightside clouds on hot Jupiters



Gao et al. (2020)



Lee et al. (2016)

Lessons from models and retrieval

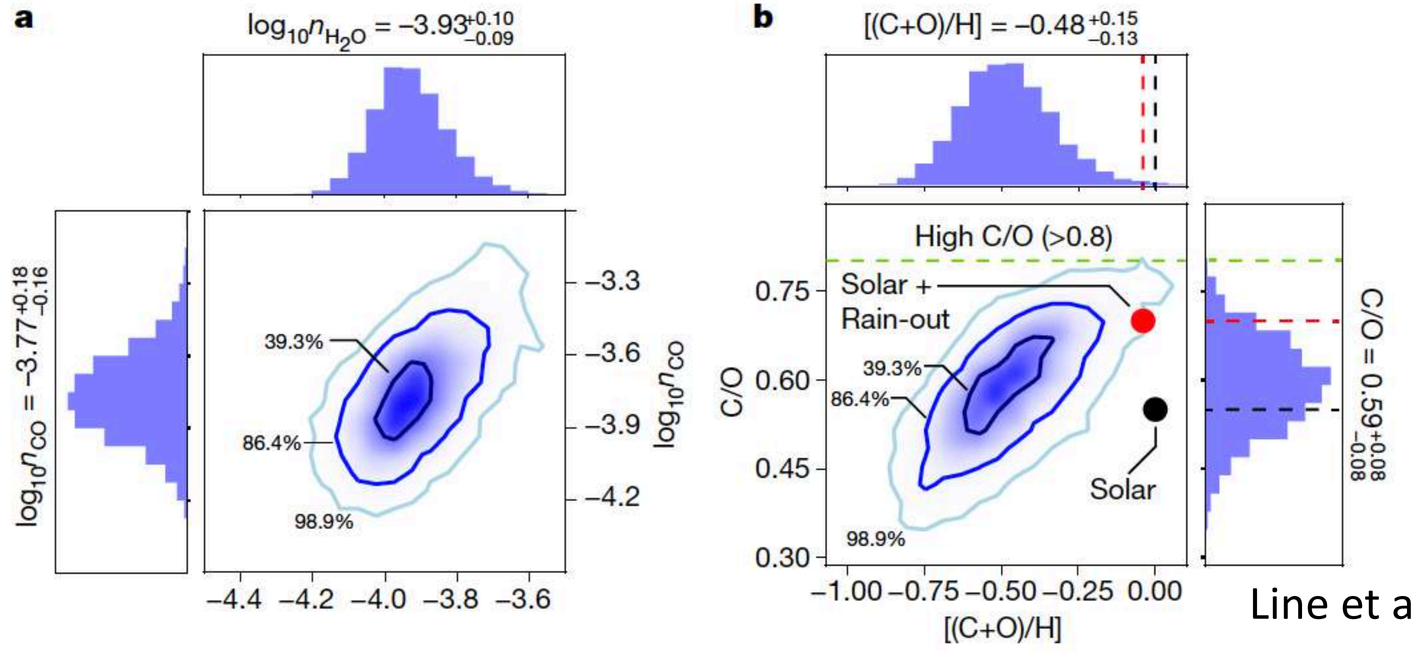
2) Relative vs absolute measurements

$$C/O \approx \frac{[CO]}{[H_2O]+[CO]} = \frac{1}{\frac{[H_2O]}{[CO]}+1}$$ (warm planets)

→ relative measurement

$$\text{metallicity} \approx [H_2O]/\,[H_2O]_{solar}$$

→ absolute measurement



Line et al. 2021

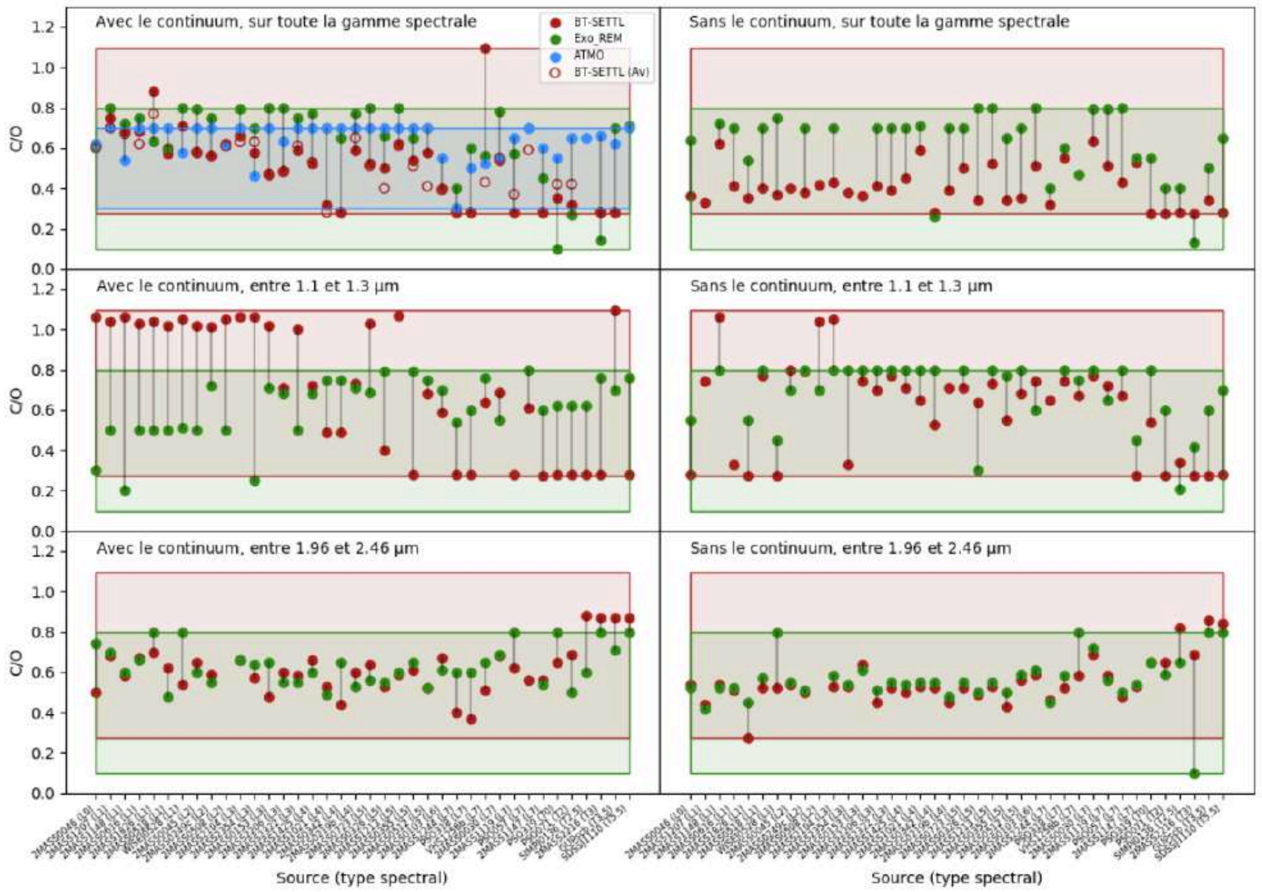
Correlation between $[H_2O]$ and [CO]: C/O must be derived directly as posterior
Uncertainty on C/O smaller than on metallicity

Relative measurements are more accurate than absolute measurements

Lessons from models and retrieval

2) Relative vs absolute measurements

Comparison of retrieved parameters (BT-Settl & Exo-REM grids)
for brown dwarfs observed with X-Shooter (R=4000)

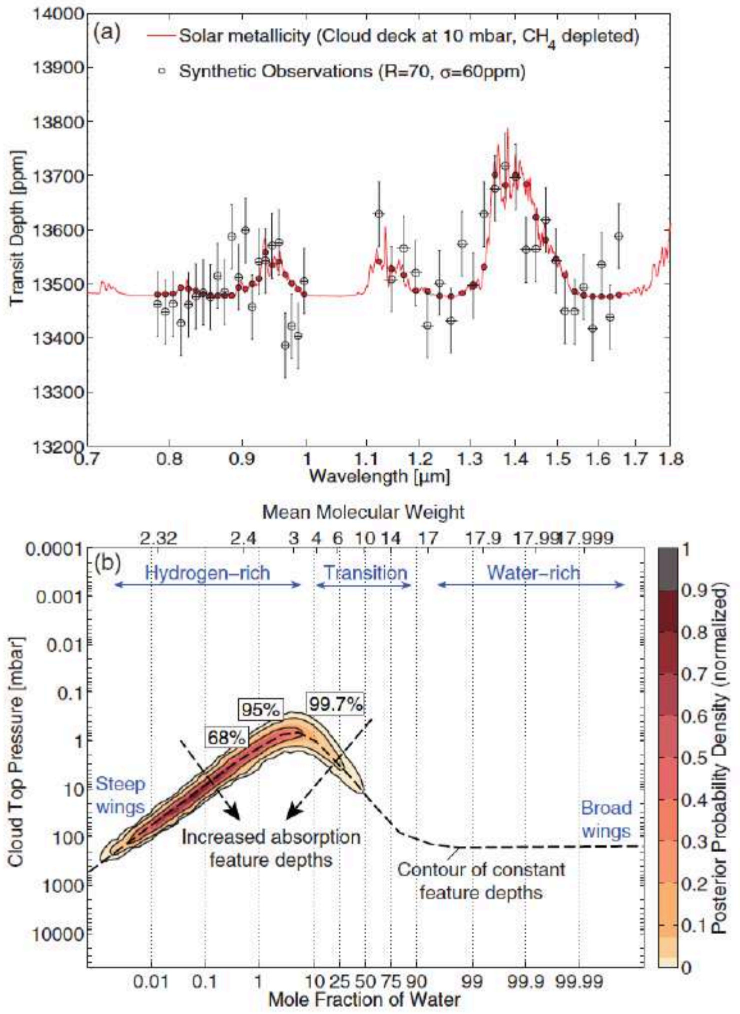


Petrus et al. *in prep*

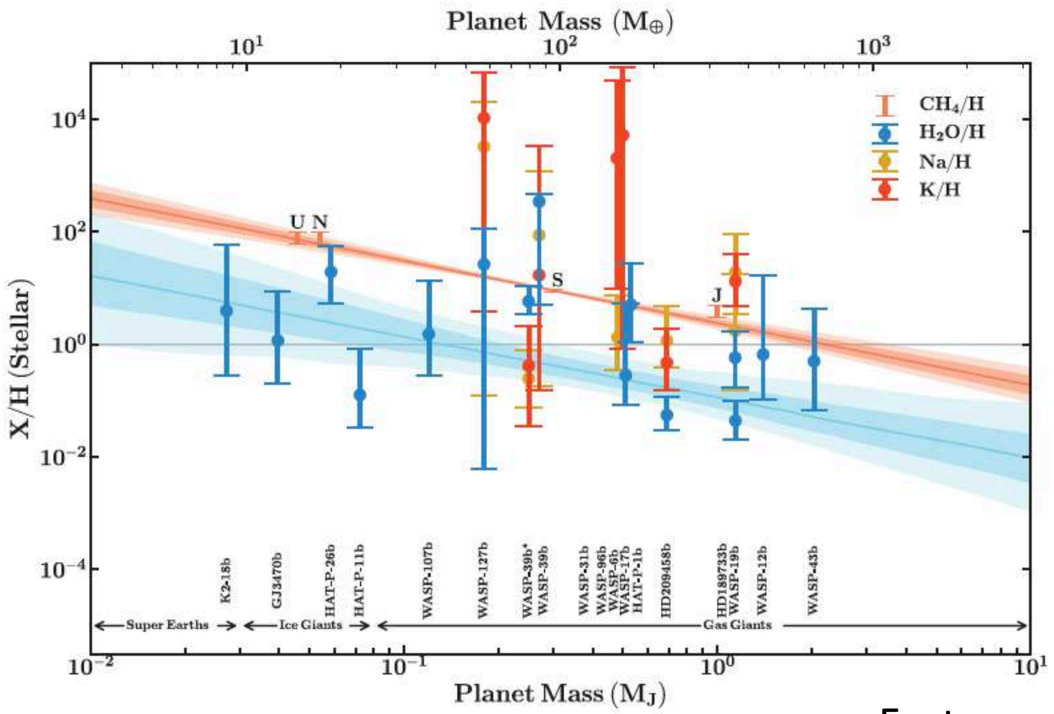
Removing the continuum + renormalisation can improve the C/O determination at medium/high resolution (elimination of biases from models and observations)

Lessons from models and retrieval

3) Biases: metallicity/cloud



Line & Seager 2013



Fortney et al. 2022

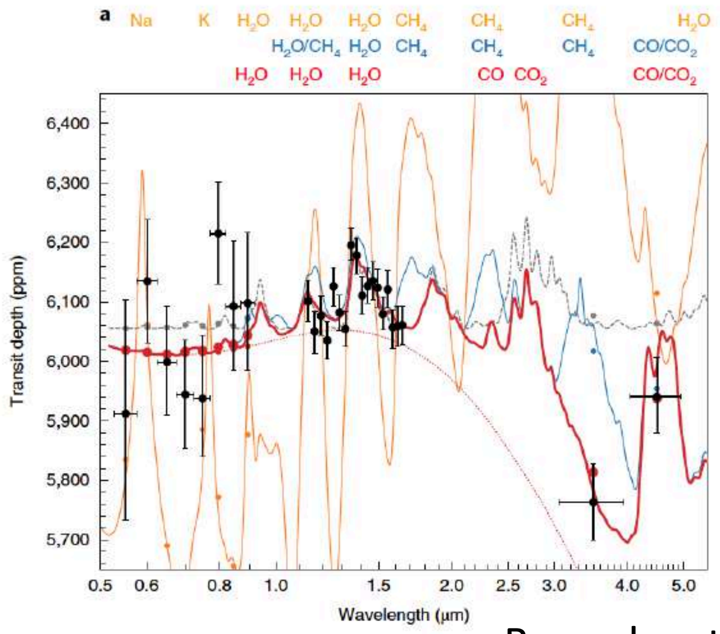
Lessons from models and retrieval

3) Biases: metallicity/cloud

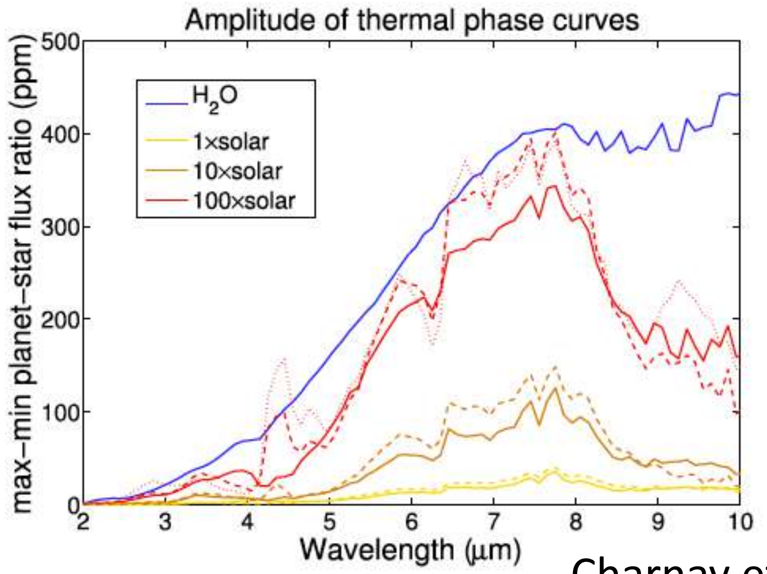
<u>How to probe cloudy/hazy atmospheres ?</u>

1) Large spectral coverage (JWST, Ariel)
2) High-resolution spectroscopy (VLT-CRIRES, SPIRou, ELT-ANDES)
3) Thermal phase curves (JWST, Ariel)

HST+Spitzer spectrum of GJ 3470 b

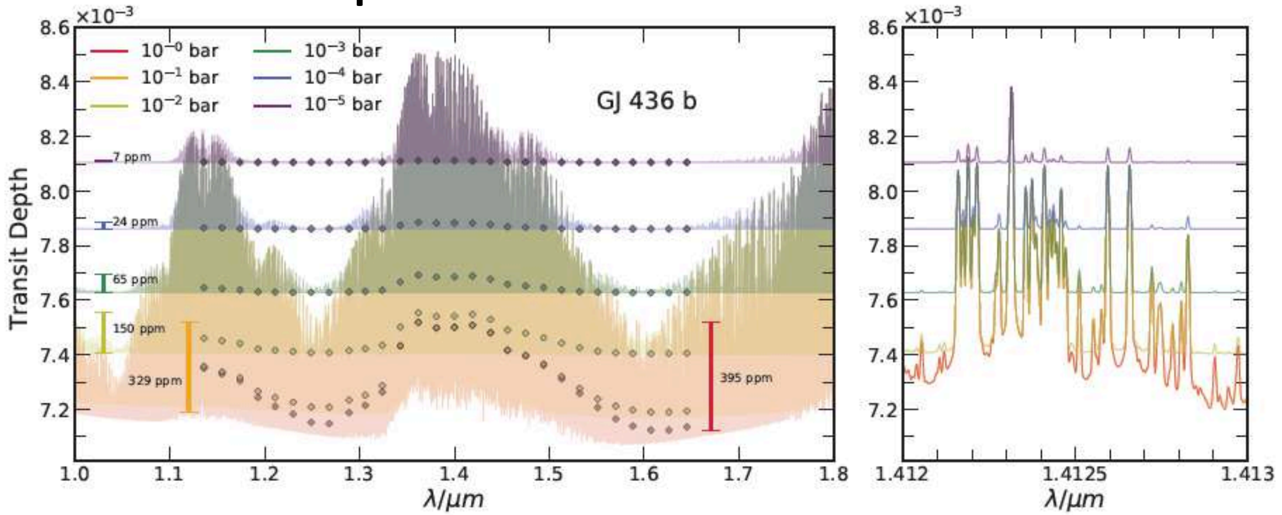


Benneke et al. 2018



Charnay et al. 2015

HR spectrum of GJ 436b

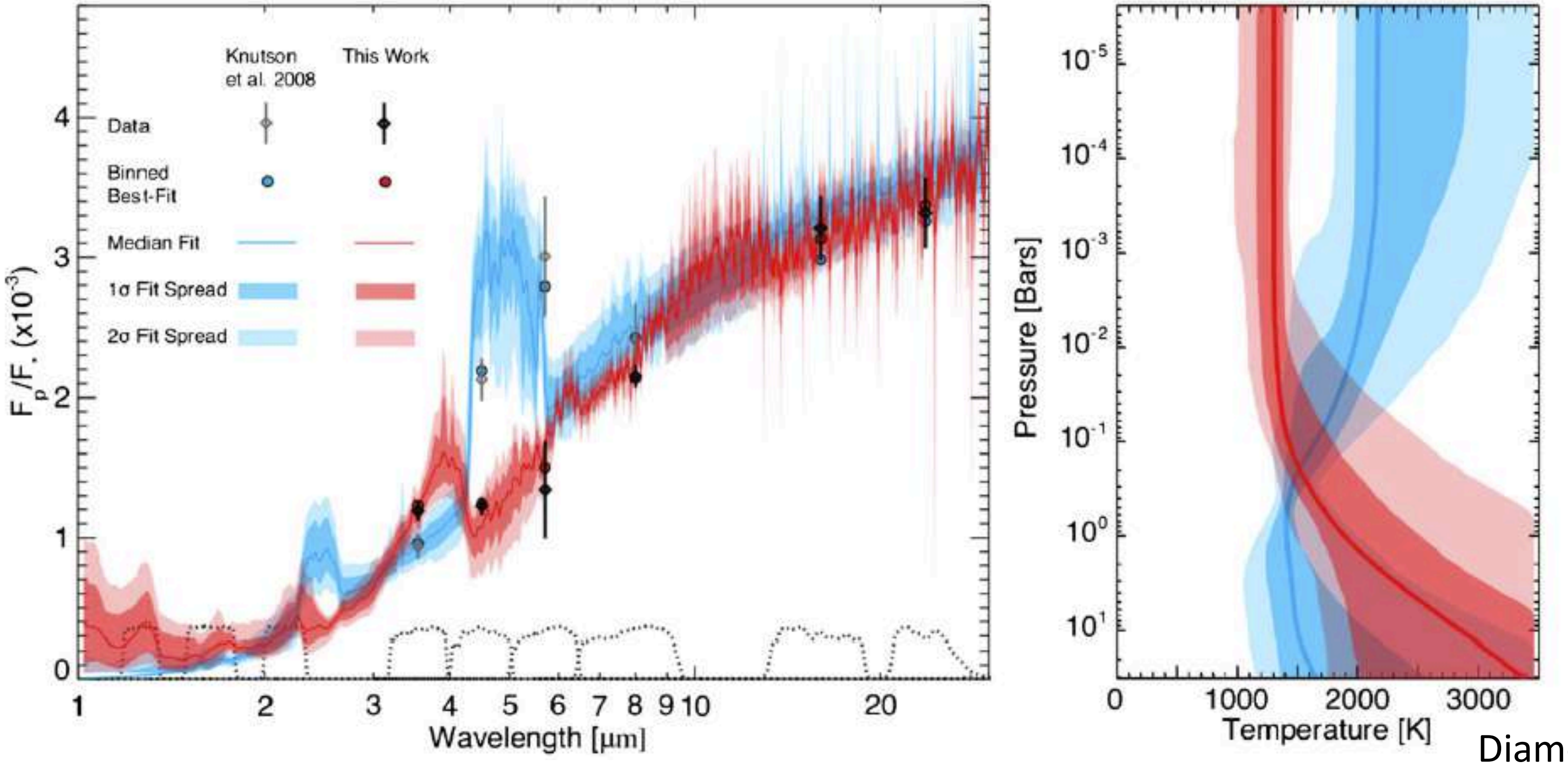


Gandhi et al. 2020

Lessons from models and retrieval

4) Biases: thermal inversion

- Detection of a stratospheric thermal inversion on HD209458 b from Spitzer eclipses (Knutson et al. 2007)
- Two classes of hot Jupiters with a transition at $T_{day} \sim 1600$ K (Fortney et al. 2008)
- Thermal inversion ruled-out after reanalysis of Spitzer data (Diamond-Lowe et al. 2014)



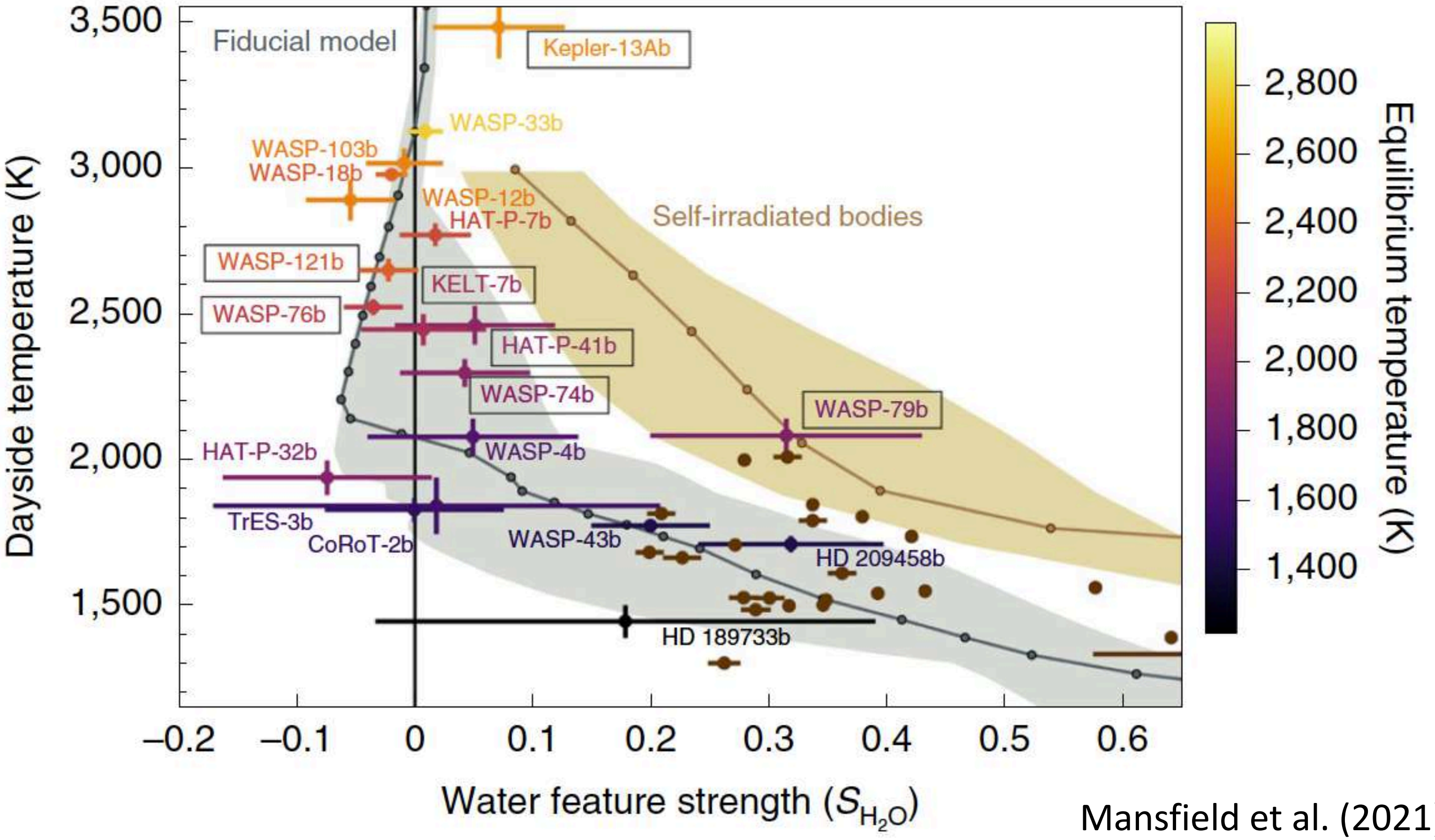
Diamond-Lowe et al. (2014)

Strong impact of instrumental systematics on retrieval

Lessons from models and retrieval

4) Biases: thermal inversion

Evolution of the water feature in eclipses

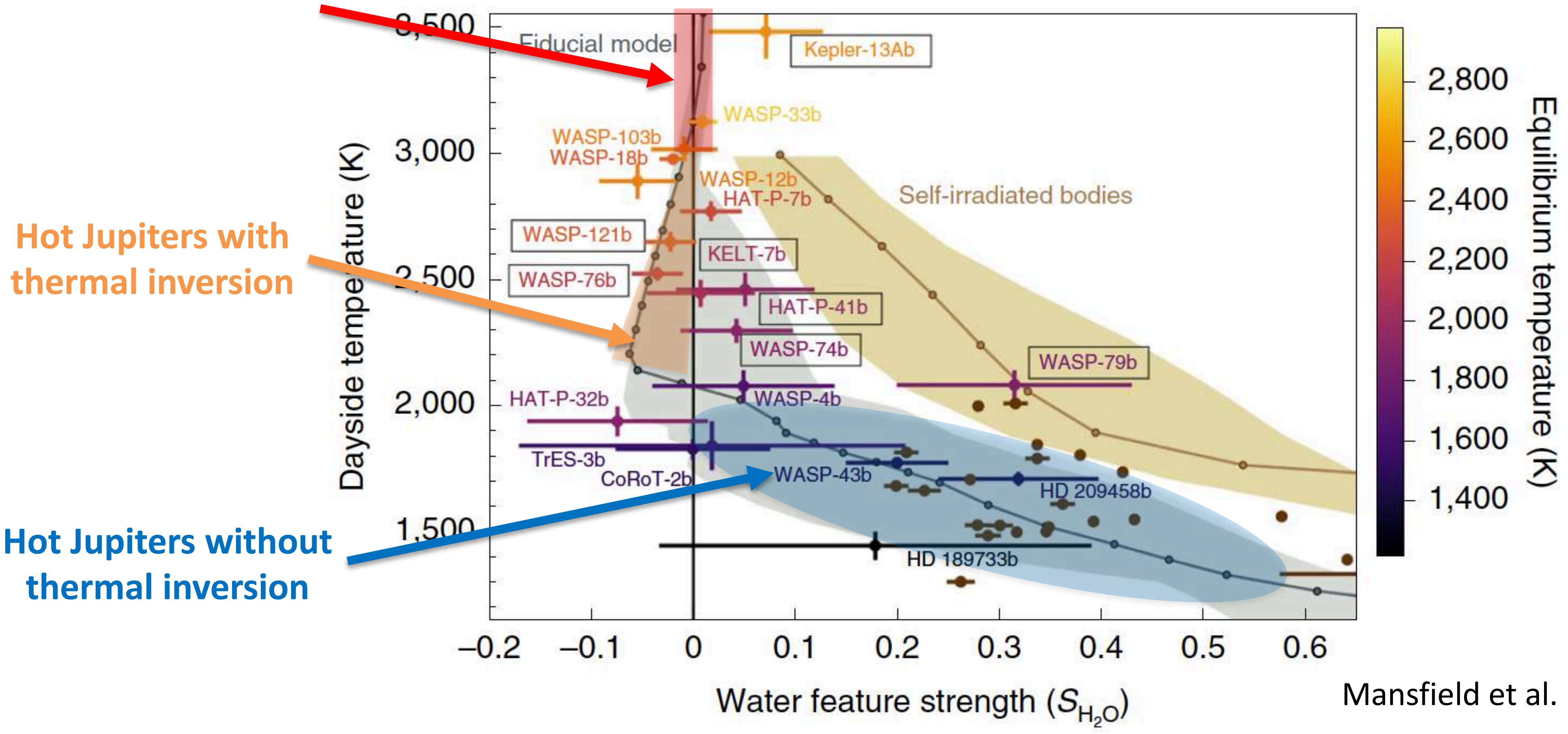


Mansfield et al. (2021)

Lessons from models and retrieval

4) Biases: thermal inversion

Evolution of the water feature in eclipses



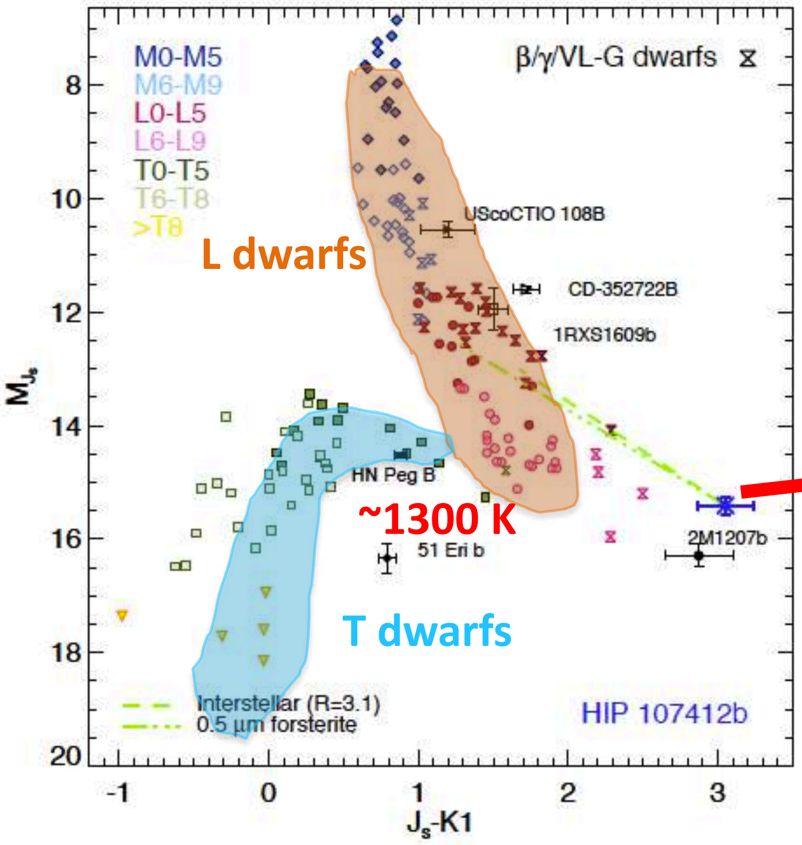
Mansfield et al. (2021)

Thermal inversions appear at higher temperatures ($T_{day} \sim 2000$ K) than initially thought

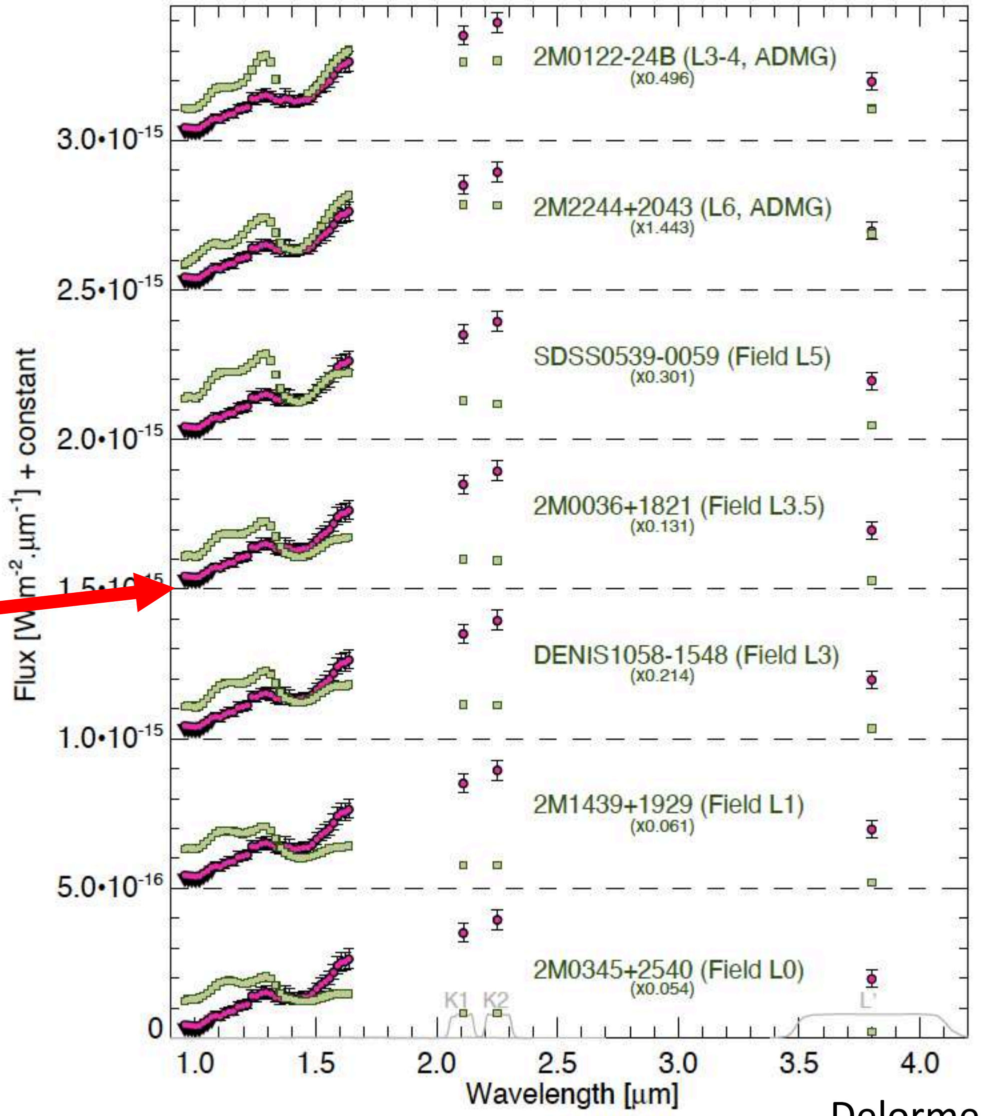
Lessons from models and retrieval

4) Biases: isothermal/clouds

Reddening of L dwarfs



HD206893 b's spectrum = almost a black body



Delorme et al. (2017)

Lessons from models and retrieval

4) Biases: isothermal/clouds

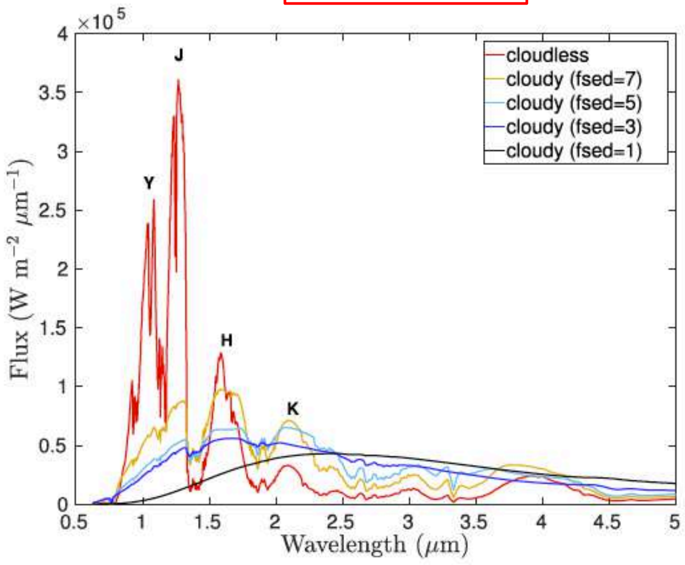
How to reduce spectral features in emission spectra ?

Lessons from models and retrieval

4) Biases: isothermal/clouds

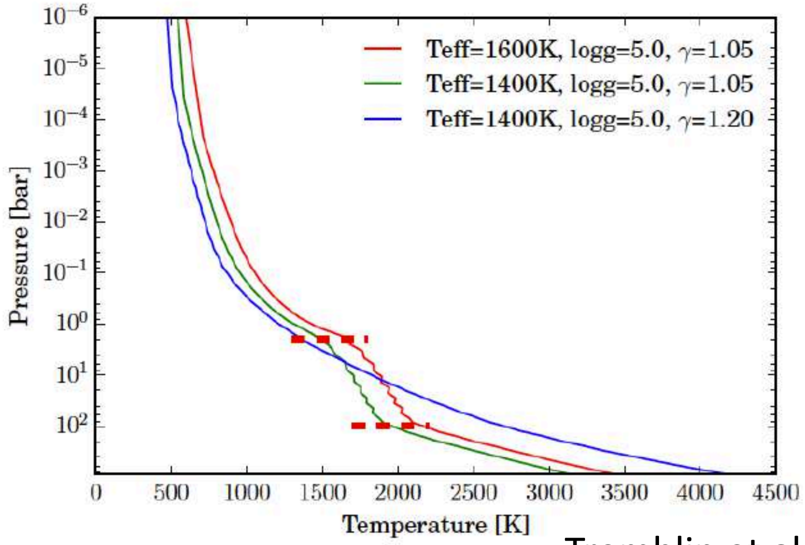
How to reduce spectral features in emission spectra ?

Clouds



Charnay et al. (2018)

Reduced thermal gradient

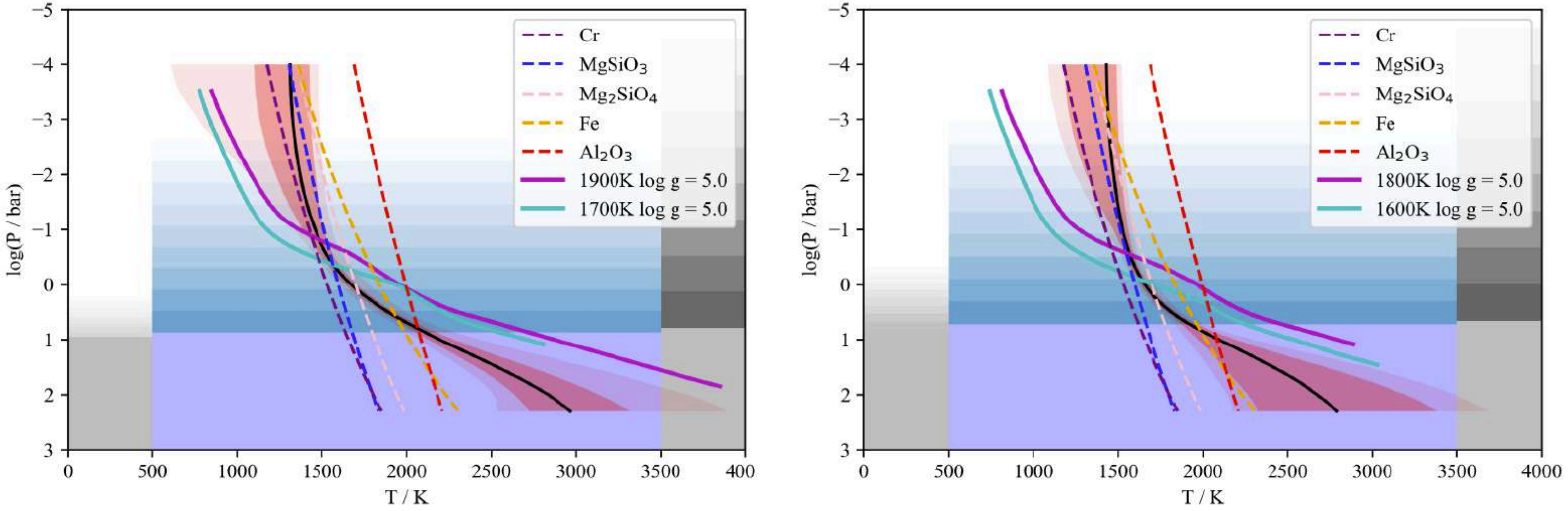


Tremblin et al. (2017)

Lessons from models and retrieval

4) Biases: isothermal/clouds

Atmospheric retrieval of two L dwarfs by Burningham et al. (2017):



Both clouds + reduced thermal gradient !

But the retrieval might be biased by its relatively simple cloud model

Lessons from models and retrieval

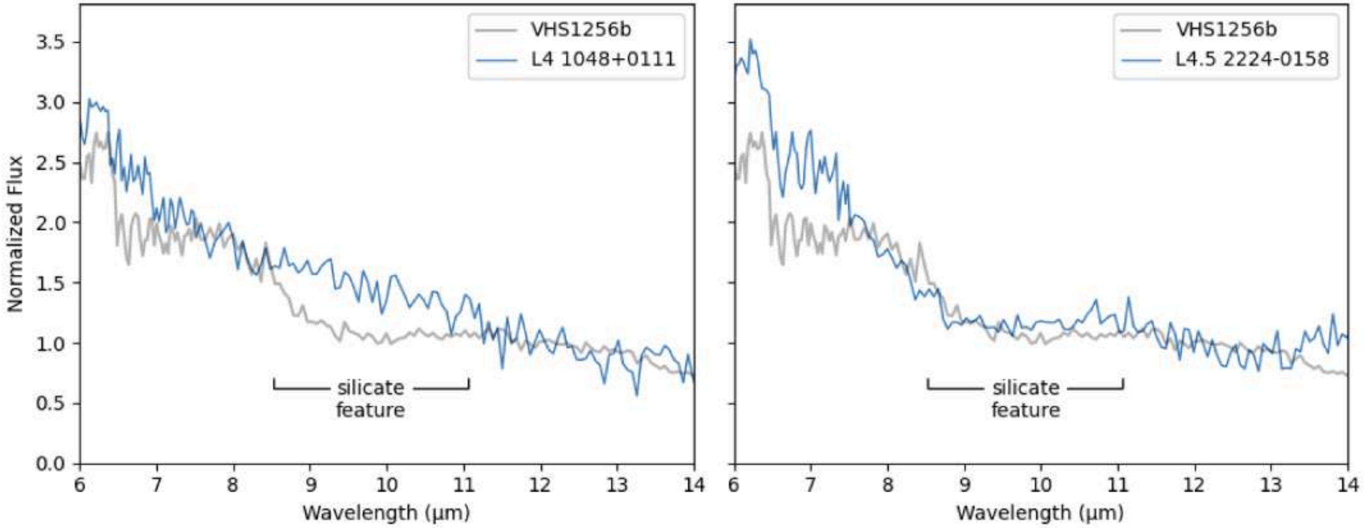
4) Biases: isothermal/clouds

<u>How to break degeneracis between clouds and reduced thermal gradient ?</u>

1) Cloud absorption features

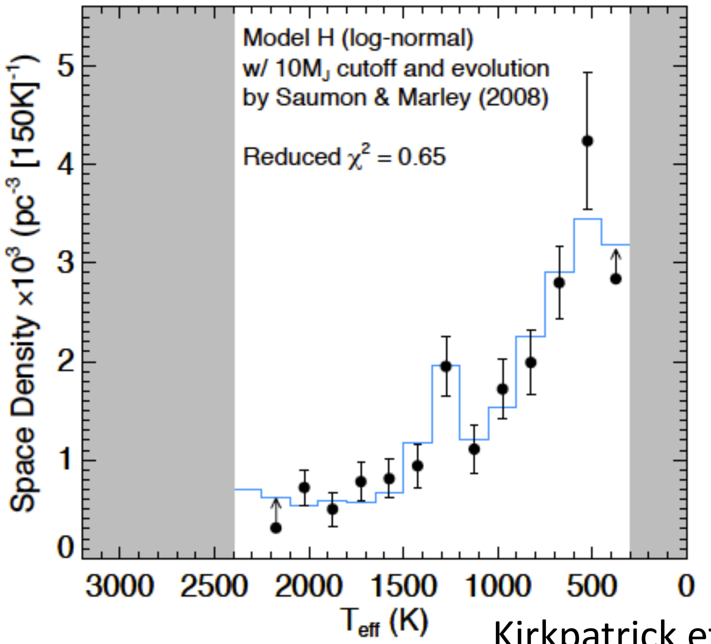
2) Thermal evolution

Silicate feature on VHS 1256 b



Miles et al. (2022)

Excess of BD at the LT transition



Kirkpatrick et al. (2020)

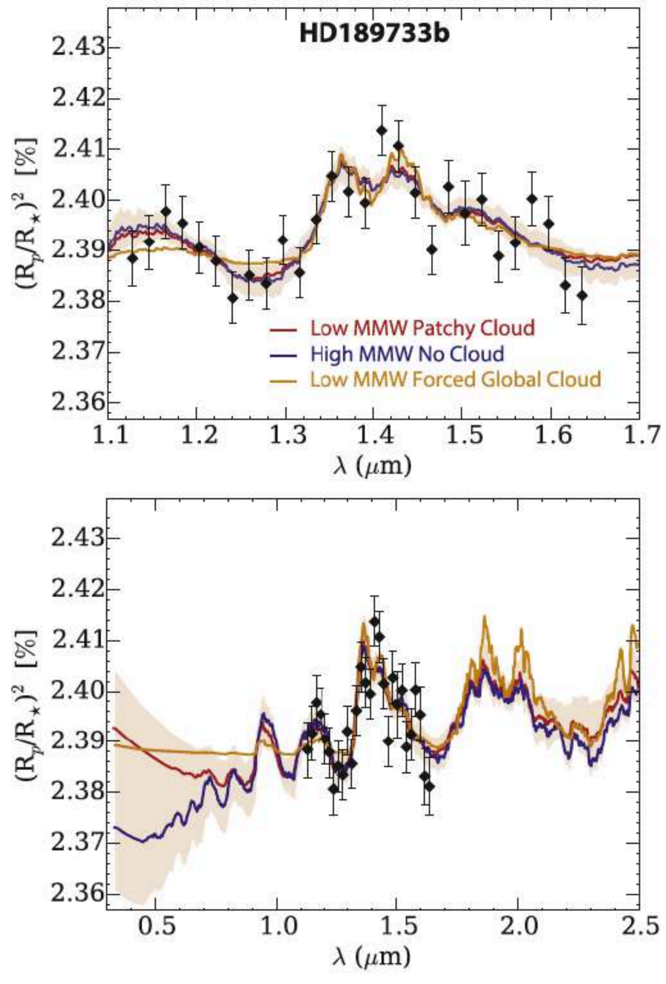
<u>But:</u>

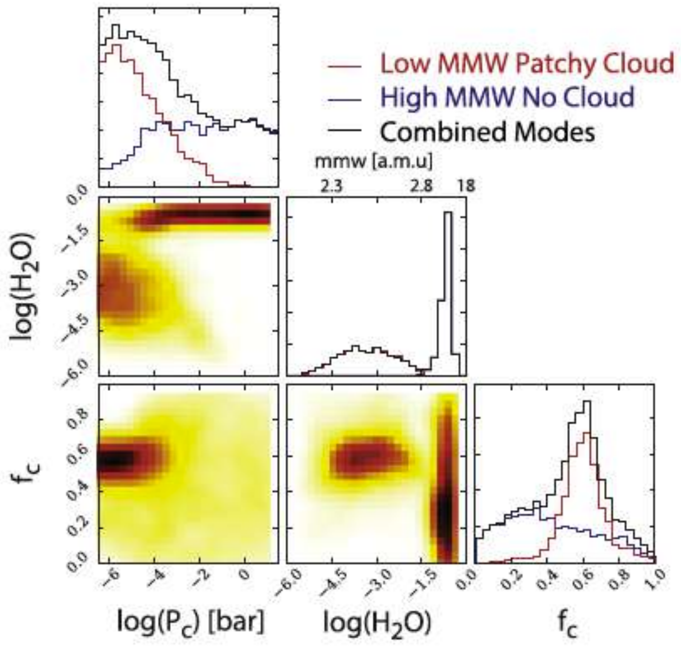
1) Clouds can be a mixture of species (e.g. Jupiter's clouds)
2) Best et al. 2020 found a minimum of BD at the LT transition

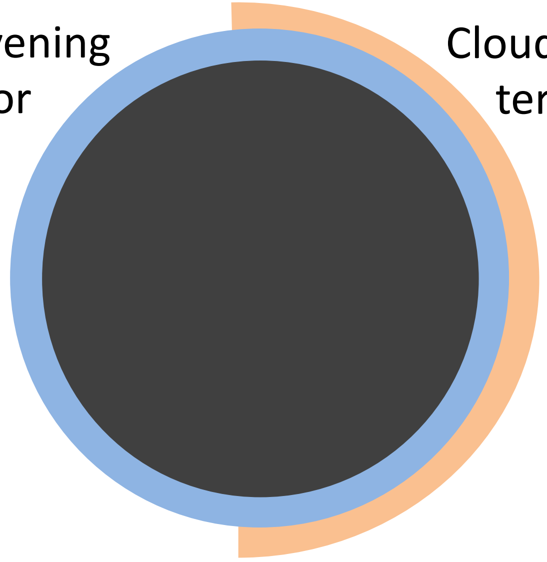
Lessons from models and retrieval

5) Biases: 3D structure

Inhomogeneous cloud cover







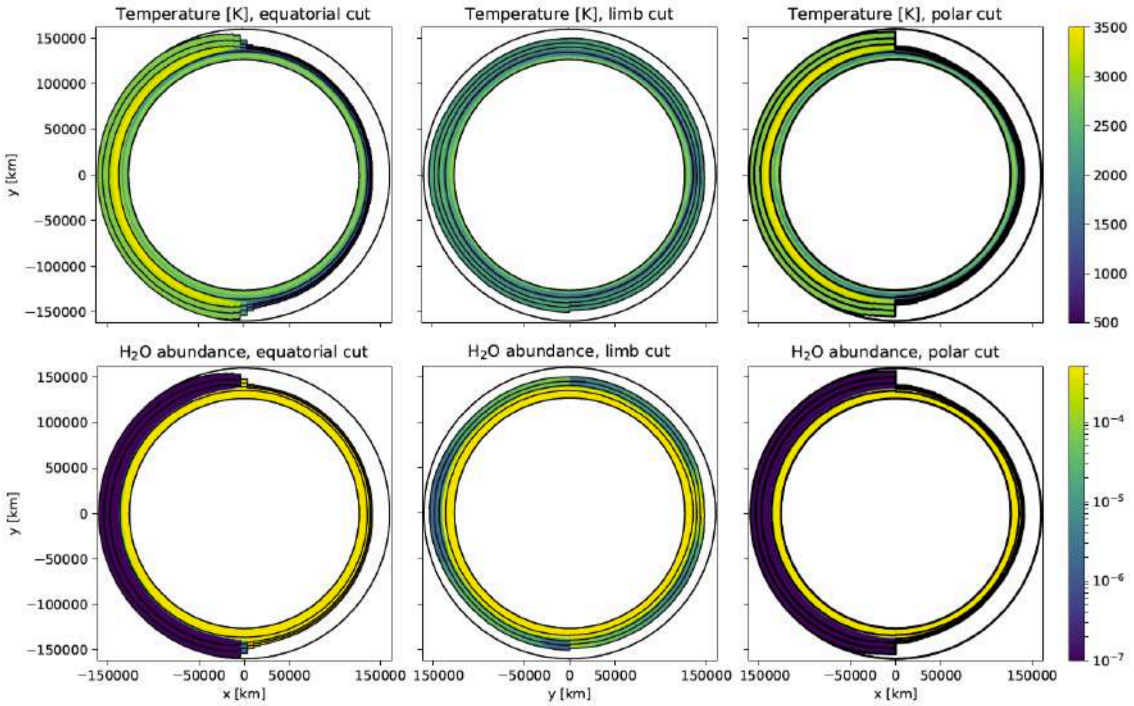
Retrieval with cloud fraction:
Degeneracy between clouds and metallicity
→ need measurements of Rayleigh slope or HR spectroscopy

Line & Parmentier (2016)

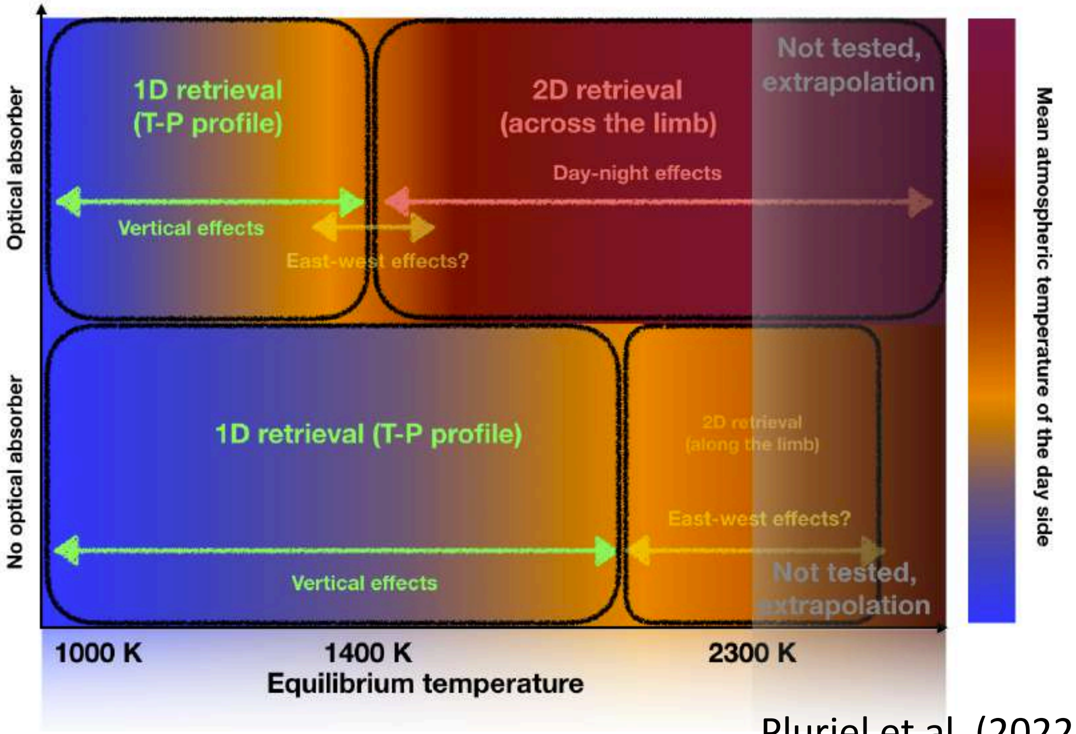
Lessons from models and retrieval

5) Biases: 3D structure

Day-night chemical heterogeneities

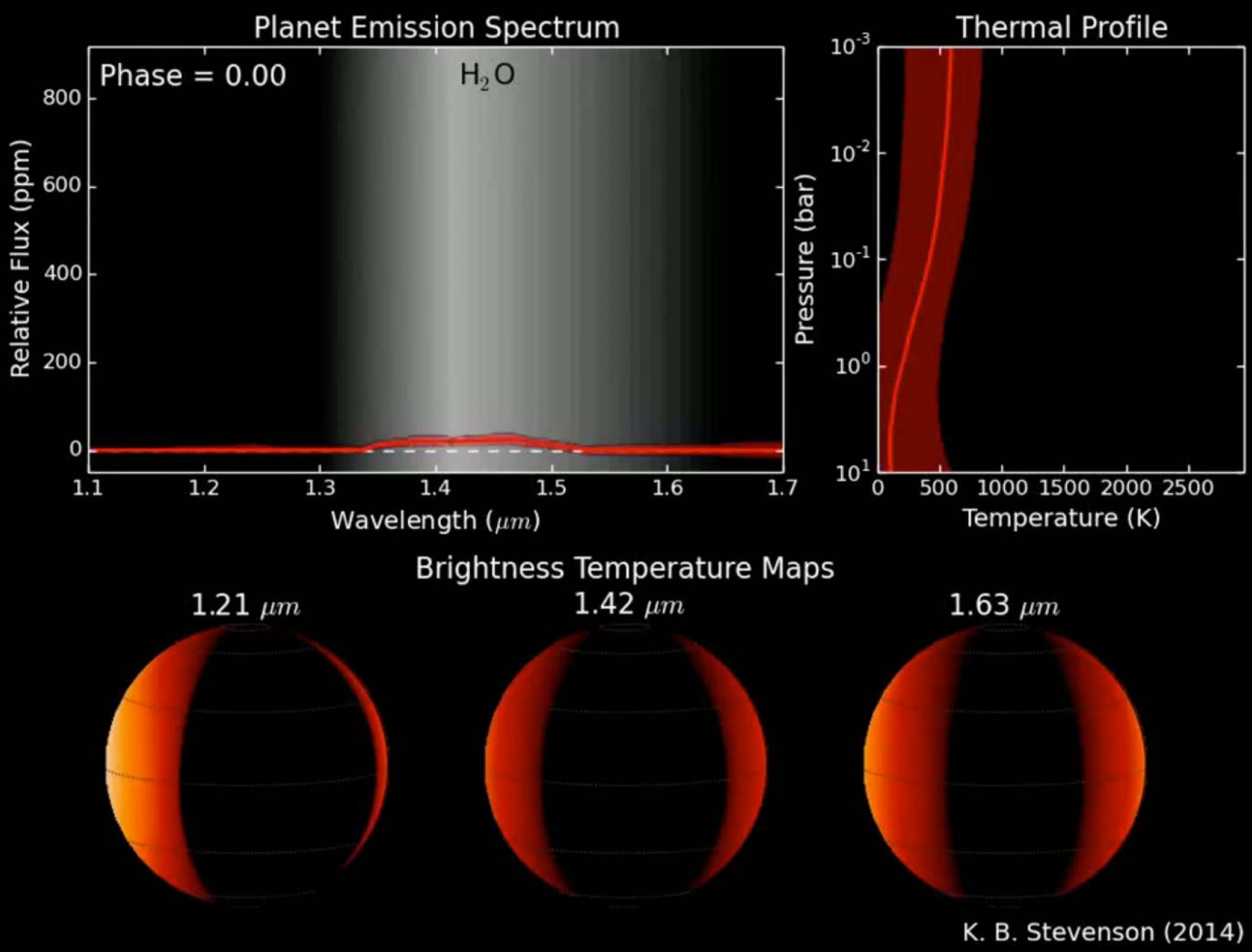


Pluriel et al. (2020)



Pluriel et al. (2022)

- Measurements of C/O can be biased by chemical heterogeneities
- Chemical disequilibrium limits heterogeneities except at high temperature
- Phase curves can be used to map horizontal variations



Planet Emission Spectrum
Phase = 0.00
H_2O
Relative Flux (ppm)
800
600
400
200
0
1.1
1.2
1.3
1.4
1.5
1.6
1.7
Wavelength (μm)
Thermal Profile
Pressure (bar)
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
0
500
1000
1500
2000
2500
Temperature (K)
Brightness Temperature Maps
1.21 μm
1.42 μm
1.63 μm
K. B. Stevenson (2014)

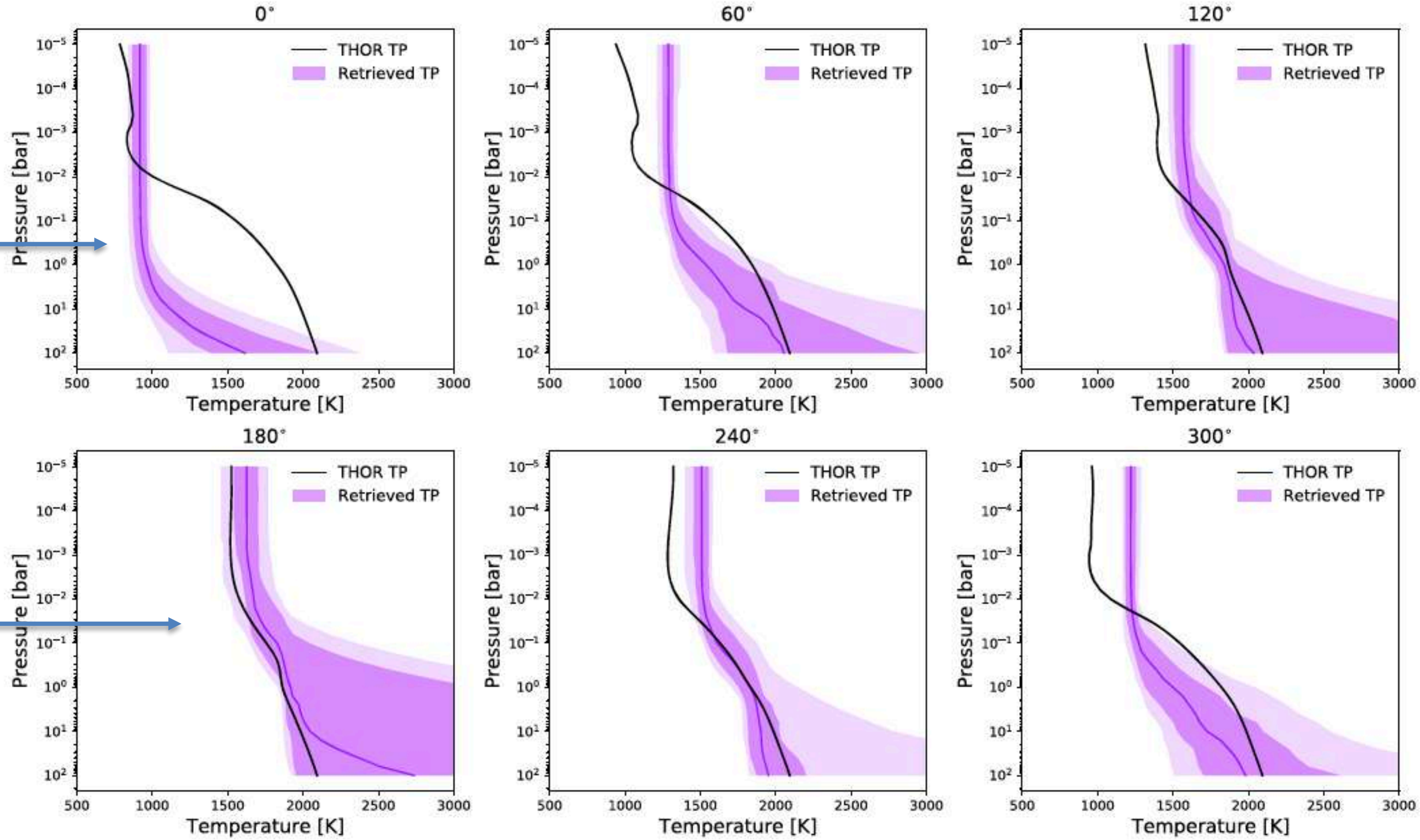
Lessons from models and retrieval

5) Biases: 3D structure

Retrieval of a simulated Ariel phase curve of WASP-43b with nightside clouds

Transit
(nightside)

Eclipse
(dayside)

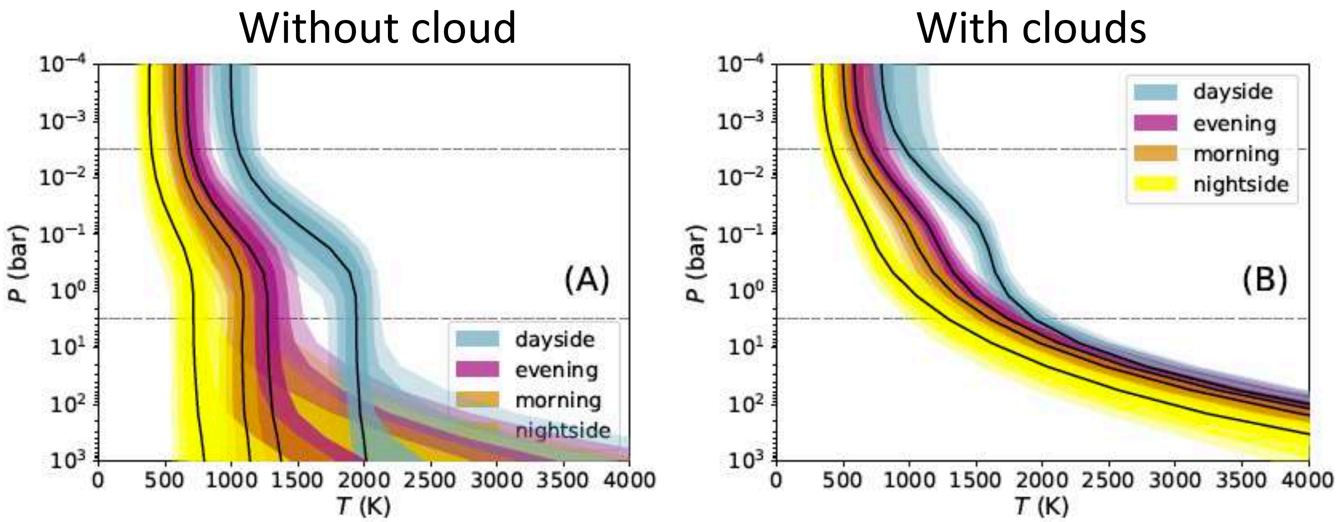


Charnay et al. (2021)

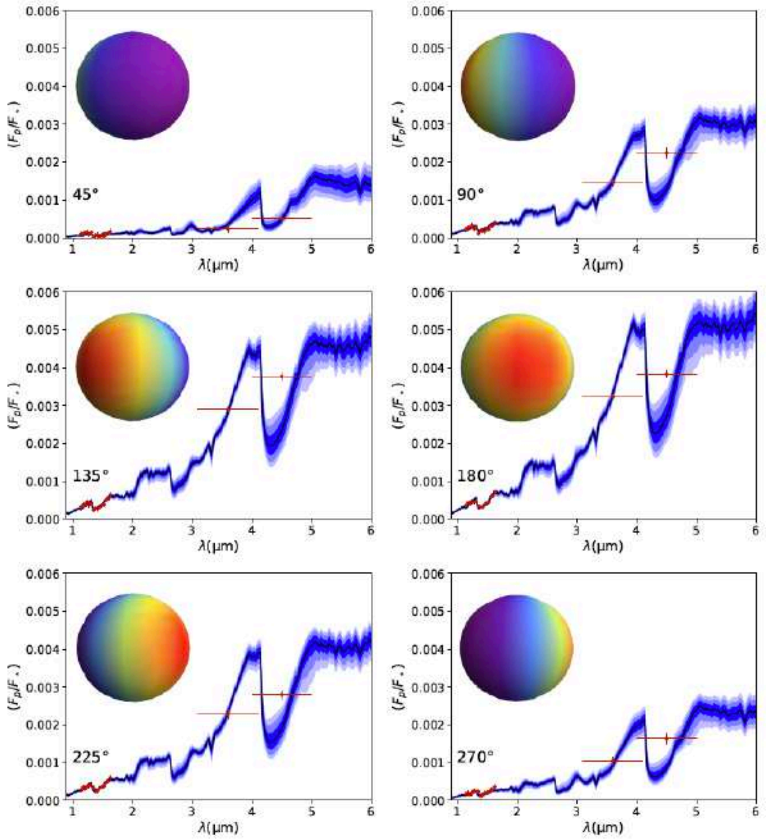
Lessons from models and retrieval

5) Biases: 3D structure

Improvement with global/2D retrieval
(e.g. Chubb & Min 2022, Irwin et al. 2019, Changeat et al. 2021)



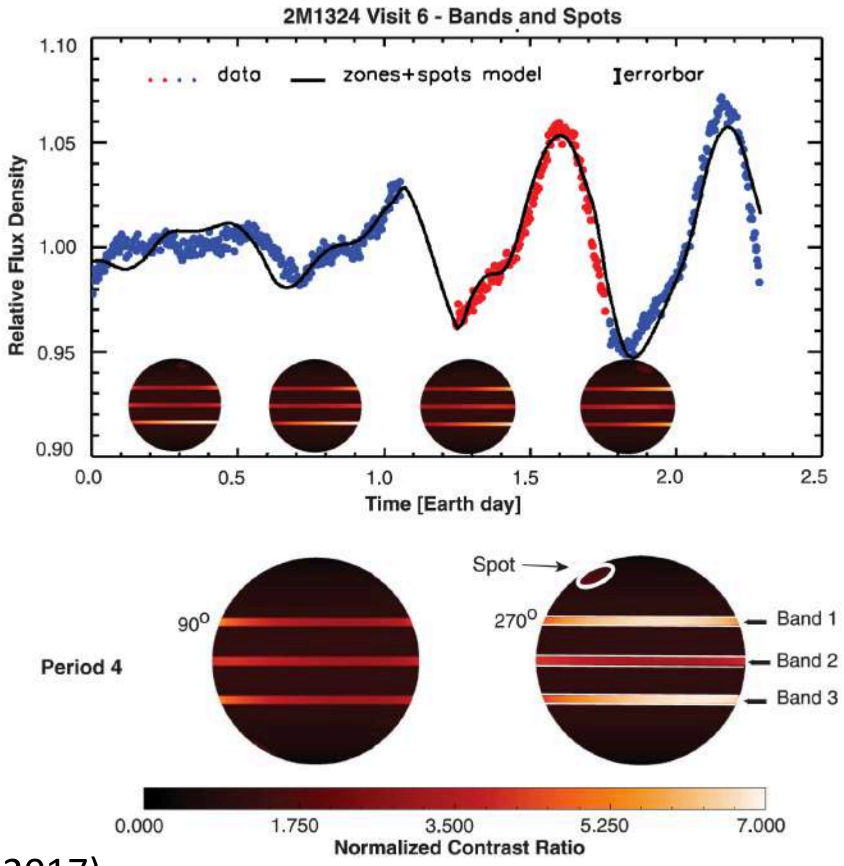
Chubb & Min (2019)



Lessons from models and retrieval

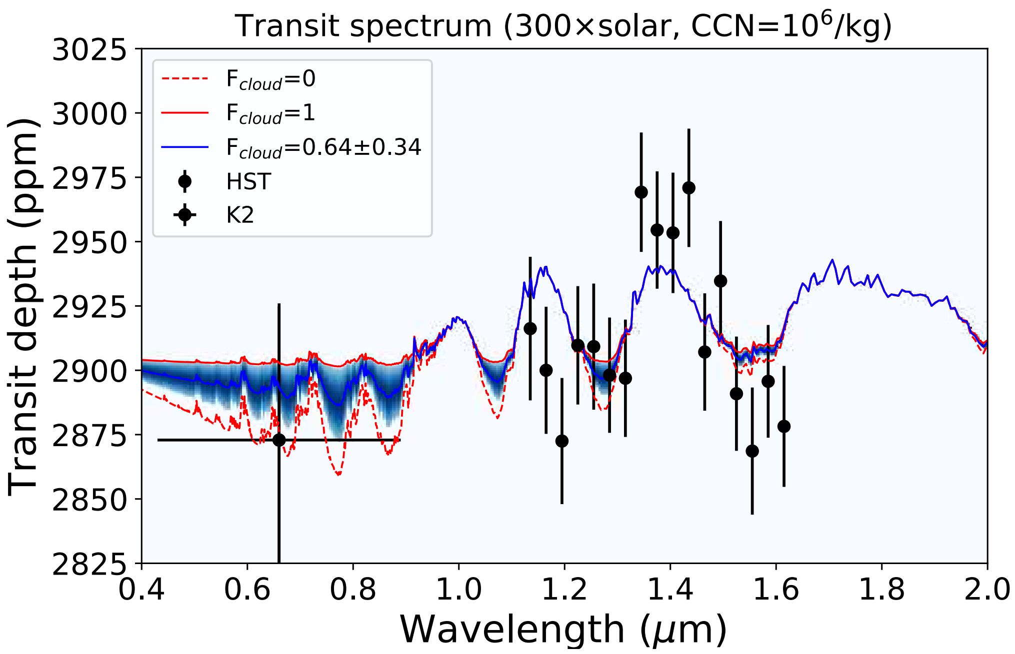
6) Biases: time-variability

Variability of a brown dwarf with Spitzer



Apai et al. (2017)

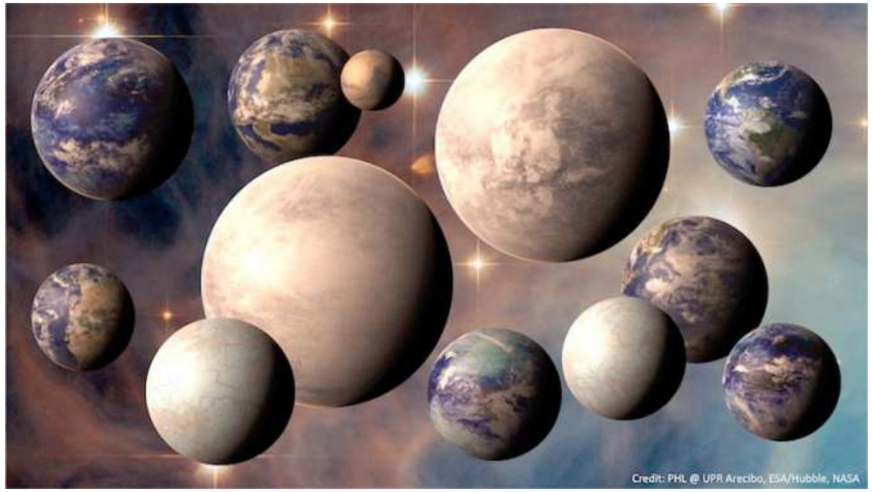
3D simulation of K2-18 b with water clouds



Charnay et al. (2021)

Possible variability of cloudiness and spectra

Take-home messages



- **We are now in the golden age of exoplanet atmospheres !**
- The different atmospheric models (self-consistent/parametric) and retrieval methods (grids, MCMC, optimisation estimation) have advantages and disavantages. **Ideally, use a combinaison of models**
- **Atmospheric models work** (at least at first order) !
- When models do not work, generally a physical process is missing or it is due to 3D effects
- The interpretation of retrieval outputs is necessary and requires **to understand the potential biases**
- **Clouds/hazes and 3D effects** are likely the largest sources of uncertainties and biases in atmospheric retrievals