
Exploring the 3D structure of ultra-hot Jupiters using ground-based high-resolution spectroscopy



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Chapter 1

Introduction

The material in this chapter is partly based on [Wardenier et al. \(2021\)](#) and

[Wardenier et al. \(2023\)](#):

- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, MNRAS, 506, 1258
- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R. (submitted to MNRAS)

1.1 New worlds around other stars

Since the discovery of the first planet around a main-sequence star other than the Sun ([Mayor & Queloz 1995](#)), the sample of known exoplanets has skyrocketed. As of April 2023, there are 5357 known planets across 3954 planetary systems – 855 of these systems host more than one planet¹. The exoplanet population displays a remarkable diversity, with objects ranging from lava planets to water worlds, and from (ultra-)hot Jupiters to ice giants. Characterising and understanding these distant worlds – many of which do not have a counterpart in our own Solar System – sheds a fundamental light on our position in the universe.

Figure 1.2 shows the sample of known exoplanets across parameter space. The vast majority of objects have been discovered using two (indirect) techniques: (i) the transit method and (ii) the radial velocity technique. For a comprehensive overview of all detection methods, see [Fischer et al. \(2014\)](#).

The transit method (e.g., [Mandel & Agol 2002](#); [Deeg & Alonso 2018](#)) relies on a planet passing in front of its host star as seen from the Earth. This results in a temporary and periodic decrease in the apparent brightness of the star. To date, the most prolific transit survey has been the Kepler mission ([Koch et al. 2010](#); [Borucki et al. 2011](#); [Batalha et al. 2013](#)), which monitored 150,000 stars over a window of four years. However, because the mission was limited to observing faint stars, the Kepler planets are not the best targets for atmospheric characterisation. One of Kepler’s successors is the TESS mission, which is performing an all-sky survey in a field that is 400 times larger ([Ricker et al. 2015](#); [Huang et al. 2018](#)). Examples of ground-based transit surveys are WASP ([Pollacco et al. 2006](#), [Butters et al. 2010](#)), KELT ([Pepper et al. 2007](#)), and MASCARA ([Talens et al. 2017](#)), which rely on multiple smaller robotic telescopes. Both TESS and the ground-based surveys focus on the brightest stars, which host the planets most suitable for atmospheric characterisation.

The radial velocity technique (e.g., [Mayor & Queloz 1995](#); [Wright 2018](#)) monitors the spectrum of a star at high resolution. If the star is orbited by a planet, it will undergo a gravitational “wobble”, causing its radial velocity (RV) to change periodically. This leads to an observable Doppler shift in the absorption lines of the stellar spectrum. RV measurements can only be performed from the ground, as they require large and heavy spectrographs. To date, most RV discoveries have been made by HARPS in La Silla ([Pepe et al. 2000](#)) and HIRES on the Keck Telescope ([Vogt et al. 1994](#)). An upcoming RV survey is the Terra Hunting experiment with HARPS3 on the Isaac Newton Telescope ([Thompson et al. 2016](#); [Hall](#)

¹Source: exoplanet.eu/catalog/

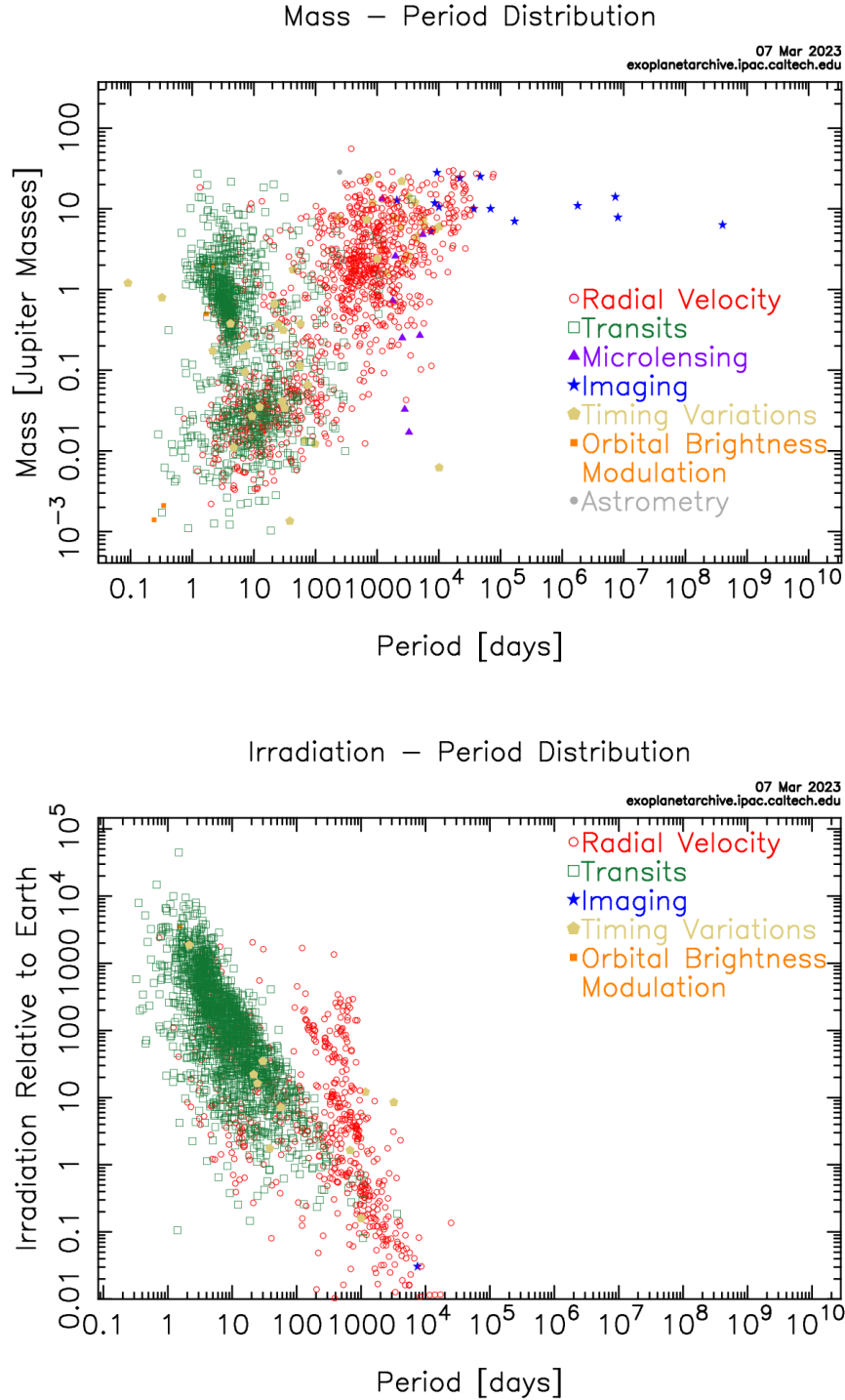


Figure 1.1: The population of confirmed exoplanets as of 7 March 2023. The plots show planet mass (top panel) and irradiation relative to Earth (bottom panel) as a function of orbital period. Different markers indicate the various detection techniques through which the planets were discovered. Plots courtesy of the NASA Exoplanet Archive (exoplanetarchive.ipac.caltech.edu/exoplanetplots/).

et al. 2018). It will look at a set of G and K dwarfs over an uninterrupted period of ten years. Such long cadences will allow for the discovery of potential Earth-analogs, which only imprint a ~ 10 cm/s Doppler shift on the spectra of their host stars.

As illustrated in Figure 1.2, each detection method is biased towards a particular region in parameter space. Both the transit method and the radial velocity technique are most sensitive to massive planets at short orbital distances from their star. This is because large, close-in planets cause the strongest brightness dips (typically 1-2%) and the strongest Doppler signals (typically ~ 100 m/s), with the periodicity of the signal being just a few days. Also, the transit method can only detect planets with an edge-on alignment – the smaller the planet and the longer its orbit, the smaller the probability that it passes in front of its host star (e.g., Stevens & Gaudi 2013). Because of these inherent detection biases, a large part of parameter space is currently unexplored. One of the goals of exoplanet science in the next decade is to push the “detection frontier” to smaller planets with longer orbital periods.

1.2 Ultra-hot Jupiters (UHJs)

1.2.1 General overview

In this work, we will focus on a special class of exoplanets: ultra-hot Jupiters (UHJs; Arcan-geli et al. 2018; Bell & Cowan 2018; Parmentier et al. 2018). UHJs are gas giants with sizes and masses comparable to those of Jupiter, but they are situated in extremely close (< 0.05 AU) vicinity of their host stars. As a result, their orbital periods are in the order of 1–2 days, while they receive 10^3 – 10^4 times more stellar radiation compared to the Earth (see bottom panel in Figure 1.2). Although the occurrence rate of hot and ultra-hot Jupiters around Sun-like stars is $\sim 1\%$ (e.g., Mayor et al. 2011; Wright et al. 2012; Beleznyay & Kunimoto 2022), a relatively large number have been detected, owing to the observational biases discussed in Section 1.1.

From dynamical arguments (e.g., Rasio et al. 1996; Showman & Guillot 2002), it follows that UHJs are likely to be tidally locked, having a dayside that is permanently irradiated and a nightside that is in permanent darkness. On the dayside, temperatures can typically reach 3500 K, while most nightside regions are ~ 1000 K. The temperature on the nightside is nonzero because of heat transport throughout the atmosphere – the extreme contrast in radiative forcing between day and night leads to strong winds in the order of 1–10 km/s (e.g., Tan & Komacek 2019), which redistribute energy across the planet. Generally, the wind profile of UHJs can be decomposed into two contributions: a day-to-night flow that carries material from the dayside to the nightside of the planet, and (depending on the drag conditions in the atmosphere) a super-rotating jet around the equator (Showman et al. 2008; Komacek & Showman 2016; Komacek et al. 2017; Hammond & Lewis 2021).

The large temperature difference between the dayside and nightside also gives rise to two distinct chemical regimes in UHJ atmospheres. The scorching, cloud-free dayside nearly resembles a stellar photosphere, where most molecules (e.g., H_2 , H_2O , TiO) are dissociated² and metals (e.g., Fe, Mg, Ca) occur in their atomic or ionic form. In fact, the *defining feature* of UHJs (as opposed to hot Jupiters) is that their dayside temperatures are high enough to dissociate a significant fraction of hydrogen and water, with the latter being an observable feature. On the nightside, however, the temperature is low enough for molecules to persist

²CO is a notable exception. Because of its strong triple bond, its dissociation temperature is much higher than for other molecules. The only planet hot enough to dissociate CO is KELT-9b (e.g., Kitzmann et al. 2018).

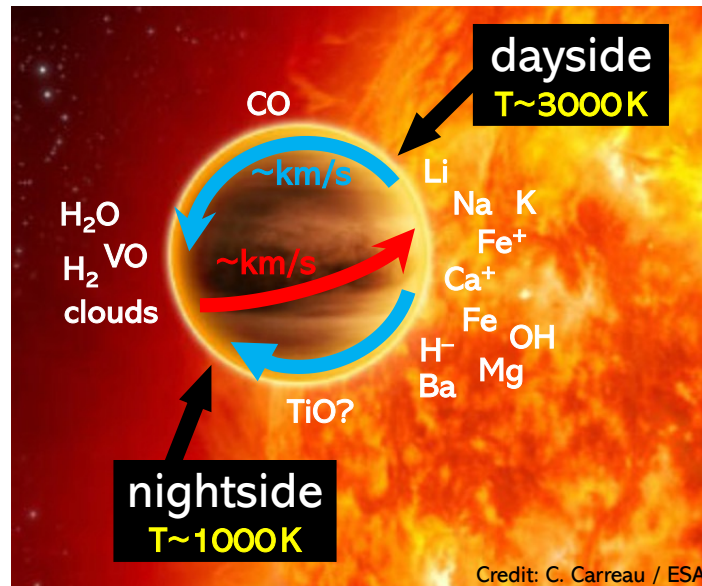


Figure 1.2: A visual summary of the discussion on ultra-hot Jupiters (UHJs) from Section 1.2. Because UHJs are tidally locked, the thermochemical structure of their atmospheres shows strong spatial variations.

and for cloud formation to occur (Wakeford et al. 2017; Helling et al. 2019, 2021; Parmentier et al. 2021; Komacek et al. 2022). Examples of hypothesised cloud species are MgSiO_3 (enstatite), Mg_2SiO_4 (forsterite), and Al_2O_3 (corundum).

1.2.2 Motivations for studying ultra-hot Jupiters

UHJs are of scientific interest for a number of reasons.

Firstly, UHJs are the best targets for atmospheric characterisation, owing to their short orbital periods, “puffy” atmospheres³, and high intrinsic brightness. This makes them amenable to transmission spectroscopy (e.g., Casasayas-Barris et al. 2018; Hoeijmakers et al. 2019; Ehrenreich et al. 2020), emission spectroscopy (e.g., Pino et al. 2020; Line et al. 2021; Brogi et al. 2023), and phase-curve studies (e.g., Arcangeli et al. 2019; Mikal-Evans et al. 2022; Coulombe et al. 2023). Additionally, the daysides of UHJs are cloud-free, providing easy observational access to the chemical inventory of their atmospheres.

Secondly, UHJs offer a unique opportunity to study atmospheric physics and chemistry under conditions that do not prevail on any of the objects in our own Solar System. Observing UHJs allows to test fundamental theories about heat transport (e.g., Bell & Cowan 2018), atmospheric dynamics (e.g., Tan & Komacek 2019), and atmospheric escape (e.g., Murray-Clay et al. 2009). One such theory concerns heat transport resulting from H_2 dissociation/recombination, whereby H_2 dissociates on the dayside, gets advected across the terminator, and recombines on the nightside. Models predict that this process should lead to stronger day-night temperature contrasts compared to cooler gas giants (Bell & Cowan 2018; Komacek & Tan 2018; Roth et al. 2021).

Finally, the atmospheres of UHJs are Rosetta stones in the context of planet formation. Planet-formation models were initially benchmarked against the Solar System. However, the discovery of exoplanets *without* Solar-System analogs has challenged these models. To

³WASP-18b is an exception due to its high gravity, reducing the scale height of its atmosphere. It has a mass of $10.3 M_{\text{Jup}}$.

date, the precise formation mechanism of UHJs remains unknown, but there are three main theories regarding their origins: (i) in-situ formation, (ii) disk migration, and (iii) high-eccentricity migration – see [Fortney et al. \(2021\)](#) for a review. In the scenario of in-situ formation, the planet accretes all its mass in its final orbit and does not migrate after it has formed (e.g., [Bodenheimer et al. 2000](#); [Batygin et al. 2016](#)). In the other scenarios, the planet forms much further away from the star. Disk migration proposes that the planet subsequently migrates inward due to interactions with the disk, accreting material on the way to its final location (e.g., [Lin et al. 1996](#); [Heller 2019](#)). On the other hand, high-eccentricity migration proposes that the planet accretes all its mass at its original location. Then, once the disk has dissipated, the planet ends up in a highly eccentric orbit due to some dynamical interaction (e.g., [Kozai 1962](#); [Lidov 1962](#); [Fabrycky & Tremaine 2007](#)), after which tidal forces cause the orbit to shrink and become circular.

The formation and migration history of a planet are encoded in the chemical composition of its atmosphere (e.g., [Lothringer et al. 2021](#)). For example, the C/O ratio of a planet sheds light on where it formed with respect to the major snowlines (H_2O , CO, CO_2) in the disk ([Öberg et al. 2011](#); [Line et al. 2021](#)). Ratios such as K/O measure the amount of refractory compared to volatile species, and indicate whether a planet grew via solid accretion or gas accretion ([Feinstein et al. 2023](#)). Furthermore, the atmosphere’s metallicity M/H can reveal whether a planet migrated to its final location before or after disk dissipation ([Madhusudhan et al. 2014](#)). Obtaining these ratios requires tight constraints on the abundances of both refractory (Fe, K, Na, etc.) and volatile species (C, O, H, etc.) in the atmosphere. For many planets (including those in the Solar System), inferring such values is challenging, as elements (especially refractories) can be sequestered into condensates that are not detectable. However, UHJs offer the unique opportunity to measure the abundances of a wide range of species (e.g., Table 1.2), as their hot daysides preclude cloud formation: all chemical building blocks are present in the gas phase and can thus be constrained.

1.2.3 Accounting for the 3D structure of ultra-hot Jupiters

A disclaimer to the previous statement is that the inherent “3D-ness” of UHJs complicates the interpretation of their observed spectra and phase curves ([Caldas et al. 2019](#); [Lacy & Burrows 2020](#); [Pluriel et al. 2020, 2022](#); [Wardenier et al. 2021](#); [Beltz et al. 2022](#); [Falco et al. 2022](#); [Gandhi et al. 2022](#); [Savel et al. 2022](#); [Pluriel 2023](#)). Because UHJs feature strong thermochemical variations across their atmospheres, there is no guarantee that the locally measured abundance of a given species is representative of the entire atmosphere, let alone for the bulk composition of the planet. In transmission spectroscopy, for example, observations probe the terminator region of the atmosphere, where the transition from the dayside to the nightside occurs. The terminator features strong compositional gradients, so its chemical profile is very much longitude-dependent. Additionally, the nightsides of UHJs *do* feature clouds, and these carry a certain fraction of the atmosphere’s refractory content.

Over the last few years, a large number of studies have demonstrated how interpreting observations of (ultra-)hot Jupiters with 1D atmospheric models can lead to *biased* inferences, both in the case of transmission and emission spectra (e.g., [Feng et al. 2016](#), [Caldas et al. 2019](#); [Pluriel et al. 2020](#); [Taylor et al. 2020](#)). At the dawn of the JWST era, these findings are alarming – the community needs to develop a deeper understanding of the 3D structure of exoplanet atmospheres to *de-bias* observational measurements and fully leverage the high-quality data provided by JWST and ground-based observatories. Currently, a

lot of resources are spent on developing (pseudo-)3D frameworks for atmospheric retrieval (e.g., Chubb & Min 2022; MacDonald & Lewis 2022; Nixon & Madhusudhan 2022). However, these frameworks require a large set of assumptions to (i) keep them computationally tractable and (ii) prevent degeneracies between different model parameters. In this regard, it is crucial to further explore the 3D nature of exoplanets and produce well-informed priors that can be used by retrieval studies to bypass degeneracies and meaningfully interpret observations from the newest generation of telescopes.

1.3 High-resolution spectroscopy (HRS)

1.3.1 General overview

Arguably the best technique for studying the 3D structure of UHJs is ground-based high-resolution spectroscopy (HRS; Snellen et al. 2010; Brogi et al. 2012; Birkby 2018). Thanks to its ability to *resolve individual spectral lines* and perform local measurements (e.g., Gandhi et al. 2022), HRS can shed light on atmospheric physics and chemistry that are not accessible to low-resolution (i.e., HST and JWST) observations. It relies on the fact that the spectral lines of a planet undergo a (periodic) Doppler shift as it orbits the star. This allows for the planet signal to be isolated from stellar⁴ and telluric absorption lines. HRS typically involves observations with spectral resolutions $R \equiv \lambda/\Delta\lambda \gtrsim 50,000$. However, successful studies have made use of instruments with $R \sim 15,000$ (Van Sluijs et al. 2022). Table 1.1 provides a comprehensive overview of high-resolution spectrographs on telescopes around the globe. Most of these instruments were built and designed for radial-velocity searches, but they have also proven invaluable to the atmospheric characterisation of exoplanets.

Because each chemical species has its own set of absorption frequencies, HRS is sensitive to the unique spectral fingerprint of atoms and molecules. In recent years, it has enabled the unambiguous detection of a vast inventory of species in the atmospheres of UHJs. These have been summarised in Table 1.2. Observations in the optical (e.g., ESPRESSO, HARPS, and MAROON-X) mainly target the alkali and refractory content of the atmosphere, as electronic transitions in atoms and ions correspond to optical wavelengths. Molecules like TiO and VO also have spectral features in this range (e.g., Hoeijmakers et al. 2015; de Regt et al. 2022). On the other hand, observations in the infrared (e.g., IGRINS, CRIRES+, SPIRou) allow to study the volatile content of the atmosphere, as longer wavelengths are sensitive to ro-vibrational transitions in molecules such as H₂O, CO, and OH (e.g., Tennyson & Yurchenko 2012).

1.3.2 Extracting the planet signal

In HRS observations, the planet spectrum typically lies buried in stellar photon noise (that is, after removing stellar and telluric lines from the data). Only a few features are strong enough to be seen directly, with the H α line, the He triplet, the Na I doublet, and the Ca I H&K lines being notable examples (e.g., Jensen et al. 2012; Nortmann et al. 2018; Alonso-Floriano et al. 2019; Seidel et al. 2019; Tabernero et al. 2021). To recover the remaining part of the spectrum,

⁴As discussed in Section 1.1, the stellar spectrum is also subject to a Doppler shift, but this shift is a factor M_*/M_p smaller (with M_* and M_p the stellar mass and the planet mass, respectively) compared to that of the planet.

Table 1.1: Overview of ground-based high-resolution spectrographs (second column), ordered by the mirror diameter of their telescope (first column). For each instrument, the table lists the spectral resolution $R \equiv \lambda/\Delta\lambda$, which can vary per observing mode, as well as the wavelength range. For instruments that reach substantially far into the infrared, the upper wavelength limits are marked in red. Clicking an instrument name in the electronic version of this thesis directs the reader to the relevant webpage of the observatory.

Telescope (D_{mirror})	Instrument	R ($\times 10^3$)	λ Range (μm)	Reference
Keck (10 m)	HIRES	25 – 85	0.30 – 1.00	Vogt et al. (1994)
	NIRSPEC	25	0.95 – 5.50	McLean et al. (1998)
HET ^a (9.2 m)	HRS	15 – 120	0.42 – 1.10	Tull (1998)
SALT ^a (9.2m)	HRS	14 – 65	0.37 – 0.89	Crause et al. (2014)
LBT (2 $\times$ 8.4 m)	PEPSI	50 – 250	0.38 – 0.91	Strassmeier et al. (2015)
VLT (4 $\times$ 8.2 m)	UVES (UT2)	80 – 110	0.30 – 1.10	Dekker et al. (2000)
	ESPRESSO ^b	70 – 140	0.38 – 0.79	Pepe et al. (2010)
	CRIRES+ (UT3)	50 – 100	0.95 – 5.20	Follert et al. (2018)
Subaru (8.2 m)	HDS	160	0.30 – 1.00	Noguchi et al. (2002)
	IRD	70	0.97 – 1.75	Kotani et al. (2018)
Gemini-North (8.1 m)	GRACES ^c	66	0.40 – 1.00	Chene et al. (2014)
	MAROON-X ^c	82 – 88	0.50 – 0.92	Seifahrt et al. (2018)
Gemini-South (8.1 m)	IGRINS ^c	45	1.42 – 2.42	Levine et al. (2018)
Magellan 2 (6.5 m)	MIKE	65 – 83	0.34 – 0.95	Bernstein et al. (2003)
	WINERED ^c	28 – 100	0.90 – 1.35	Kondo et al. (2015)
MMT (6.5 m)	ARIES ^d	1.5 – 50	1.00 – 5.00	McCarthy et al. (1998)
DCT (4.3 m)	EXPRES	140	0.38 – 0.68	Fischer et al. (2017)
AAT (3.9 m)	HERMES	28 – 50	0.47 – 0.79	Sheinis (2016)
	VELOCE	80	0.58 – 0.93	Gilbert et al. (2018)
TNG (3.8 m)	HARPS-N	115	0.38 – 0.69	Cosentino et al. (2014)
	GIANO-B	50	0.95 – 2.45	Oliva et al. (2012)
ESO 3.6-m telescope	HARPS	115	0.38 – 0.69	Pepe et al. (2000)
	NIRPS	75 – 82	0.97 – 1.85	Wildi et al. (2017)
CFHT (3.6 m)	ESPaDOnS	68 – 81	0.37 – 1.05	Donati et al. (2003)
	SPIRou	75	0.95 – 2.35	Thibault et al. (2012)
Calar Alto (3.5 m)	CARMENES	80 – 100	0.52 – 1.71	Quirrenbach et al. (2016)
IRFT (3.0 m)	iSHELL	75	1.10 – 5.30	Rayner et al. (2016)
INT (2.5 m)	HARPS3 ^d	25 – 85	0.38 – 0.69	Thompson et al. (2016)

^a HET and SALT have a fixed elevation and can only rotate azimuthally.

^b ESPRESSO can combine the signal from all four of the VLT's unit telescopes (UTs).

^c Visiting instruments.

^d Not yet commissioned at the time of writing.

Table 1.2: Overview of chemical species for which detections have been reported in the atmospheres of UHJs. Species for which “tentative evidence” was found are not included in the table. Neutral atoms are labelled with Roman numeral I, and singly-ionised species with Roman numeral II. Planets are sorted by their equilibrium temperature $T_{\text{eq}} = T_{\text{star}} \sqrt{R/2a}$, with T_{star} the stellar effective temperature, R the stellar radius, and a the semi-major axis of the orbit, respectively. Table complete as of April 2023.

Planet (T_{eq})	Species detected with HRS
WASP-76b (2180 K)	Na I (Seidel et al. 2019), Fe I (Ehrenreich et al. 2020), Li I, Mg I, Ca II, Mn I, K I, H I, (Tabernero et al. 2021), OH (Landman et al. 2021), V I, Cr I, Ni I, Sr II, Co I (Kesseli et al. 2022), H ₂ O, HCN (Sánchez-López et al. 2022), Ba II (Azevedo Silva et al. 2022), CO, H ₂ O (Yan et al. 2023), VO, Ca I, O I, Fe II (Pelletier et al., subm.)
KELT-20b (2250 K)	Na I, H I (Casasayas-Barris et al. 2018), Ca II, Fe II (Casasayas-Barris et al. 2019), Fe I (Stangret et al. 2020), Si I (Cont et al. 2022a), Cr I (Borsa et al. 2022), Ni I (Kasper et al. 2023)
WASP-121b (2360 K)	Na I (Sindell et al. 2018), Fe I (Gibson et al. 2020), H I (Cabot et al. 2020), Cr I, V I, Fe II (Ben-Yami et al. 2020), Mg I, Ca I, Ni I, V I (Hoeijmakers et al. 2020), K I, Li I, Ca II, (Borsa et al. 2021b), Sc II (Merritt et al. 2021), Co I, Sr II, Ba II (Azevedo Silva et al. 2022), CO, H ₂ O (this thesis, see Appendix A)
WASP-18b (2400 K)	H ₂ O, CO, OH (Brogi et al. 2023)
HAT-P-70b (2560 K)	Ca II, Cr I, Cr II, Fe I, Fe II, H I, Mg I, Na I, V I (Bello-Arufe et al. 2022)
WASP-189b (2640 K)	Fe I (Yan et al. 2020), TiO, Fe II, Ti I, Ti II, Cr I, Mg I, V I, Mn I (Prinoth et al. 2022), CO (Yan et al. 2022)
WASP-33b (2780 K)	TiO (Nugroho et al. 2017), Ca II (Yan et al. 2019), Fe I (Nugroho et al. 2020), H I (Yan et al. 2021), OH (Nugroho et al. 2021), TiO (Cont et al. 2021), Si I (Cont et al. 2022a), Ti I, V I (Cont et al. 2022b), CO (Van Sluijs et al. 2022)
KELT-9b (4050 K)	H I (Yan & Henning 2018), Fe I, Fe II, Ti II (Hoeijmakers et al. 2018), Mg I (Cauley et al. 2019), Na I, Cr II, Sc II, Y II (Hoeijmakers et al. 2019), Ca II (Turner et al. 2020), O I (Borsa et al. 2021a), Si I (Ridden-Harper et al. 2023); Ca I, V I, Ti I, Cr I, Ni I, Sr II, Ba II, Tb II (Borsato et al. 2023)

however, the data must be cross-correlated with a template model that contains the lines of one or multiple species (Snellen et al. 2010). The idea behind this approach is to combine the signal from all spectral lines simultaneously and boost the signal-to-noise ratio (SNR) of the observation. The SNR resulting from cross-correlation scales with $\sqrt{N_{\text{lines}}}$, where N_{lines} is the number of spectral lines over which the operation is performed (Snellen et al. 2015). The left panel of Figure 1.3 shows the detection of CO in the atmosphere of the hot Jupiter HD 209458b – the first chemical detection in the atmosphere of an exoplanet using the cross-correlation technique. The cross-correlation function (CCF) was obtained by summing over all integrations during the transit, to maximise the signal.

HRS is not only sensitive to orbital motion. In fact, the total Doppler shift of the planet spectrum is induced by (i) the systemic velocity V_{sys} of the star, (ii) the orbital motion K_p of the planet, (iii) planetary rotation, and (iv) atmospheric dynamics. In the case of (ultra-)hot Jupiters, the last two effects correspond to velocities at the 1–10 km/s level, which means that they are measurable. Therefore, the shapes, depths, and positions of the lines in the planet spectrum can also be used to constrain wind patterns (e.g., Snellen et al. 2010; Loudén & Wheatley 2015; Flowers et al. 2019; Seidel et al. 2020), and, in some cases, rotation rates (Snellen et al. 2014; Brogi et al. 2016; Schwarz et al. 2016).

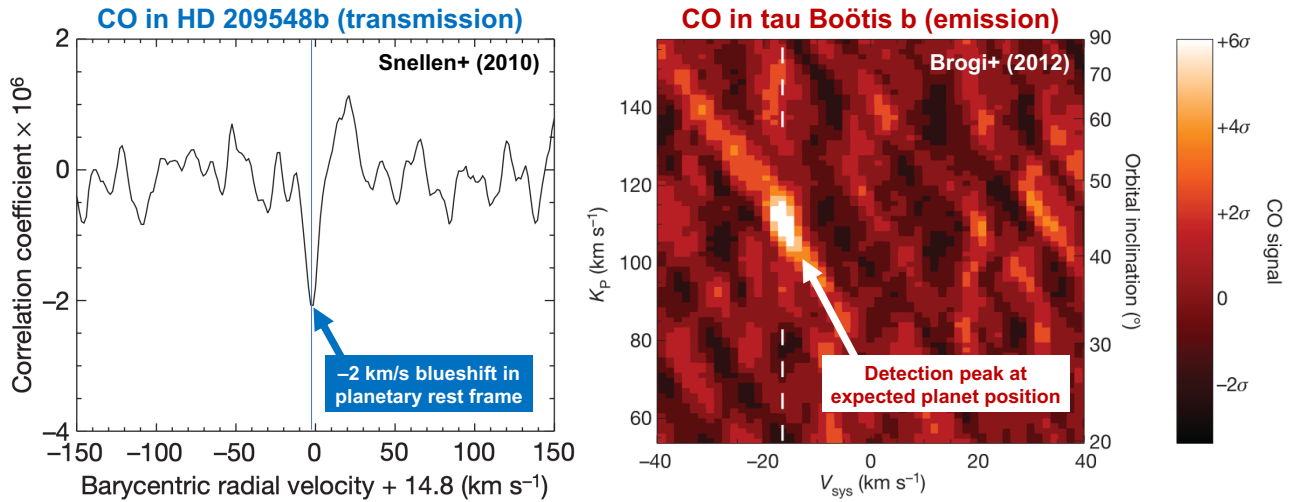


Figure 1.3: Detection of CO in the atmospheres of the hot Jupiters HD 209458b (in transmission; [Snellen et al. 2010](#)) and τ Boötis b (in emission; [Brogi et al. 2012](#)) with VLT/CRIRES. The left panel shows the cross-correlation function (CCF) aggregated over all integrations during the transit. The (negative) peak in the CCF indicates a match between the planet spectrum and the CO lines in the template model. The best match is achieved when the template is Doppler-shifted by -2 km/s in the planetary rest frame, suggesting the presence of day-to-night winds on the planet. The right panel shows a K_p - V_{sys} map, which essentially visualises the CCF for different combinations of system velocity V_{sys} and orbital velocity semi-amplitude K_p . The fact that the detection peak coincides with the known (K_p , V_{sys}) values of the planet means that the signal is of astrophysical origin. See Sections 2.3.3 and 2.3.4 for further details.

The CCF in the left panel of Figure 1.3 is plotted in the planetary rest frame, an imaginary frame that moves with the planet as it orbits the star. In the planetary rest frame, the only Doppler contributions are from rotation and dynamics. This is the reason why [Snellen et al. \(2010\)](#) attributed the “anomalous” -2 km/s Doppler shift of the CCF peak to a day-to-night flow that blueshifts the CO absorption lines⁵. This was the first wind-speed measurement made in the atmosphere of an exoplanet.

The right panel of Figure 1.3 shows the detection of CO in the non-transiting planet τ Boötis b ([Brogi et al. 2012](#)). The detection manifests as a peak in the K_p - V_{sys} map, which is an alternative way to plot the cross-correlation between the data and the template model. To produce the map, the data are multiplied with a template that is Doppler-shifted according to different (K_p , V_{sys}) combinations. In the absence of planet rotation and dynamics, the signal position should coincide with the *known* parameters of the system. In general, K_p - V_{sys} maps can be seen as a time-average over the observation, as they are based on the sum of all integrations. In Sections 2.3.3 and 2.3.4, we will discuss the cross-correlation technique and K_p - V_{sys} maps in more detail.

A final benefit of HRS is that it can probe processes in the upper atmospheres of exoplanets, such as atmospheric escape (e.g., [Murray-Clay et al. 2009](#); [Yan & Henning 2018](#)). In transmission, the strongest absorption lines (such as H α and Ca II) can even probe altitudes that extend beyond the Roche lobe, where material is no longer gravitationally bound to the planet. Numerous studies have reported extreme Doppler broadening of these absorption lines, suggesting vertical winds with velocities of tens of km/s (e.g., [Seidel et al. 2020](#), [Borsa et al. 2021b](#)).

⁵A *negative* Doppler shift implies that the absorbers are moving *towards* the observer (blueshift), while a *positive* Doppler shift implies that the absorbers are moving *away* from the observer (redshift).

1.4 Thesis outline

The goal of this thesis is to explore how the 3D structure of ultra-hot Jupiters (UHJs) impacts their high-resolution transmission spectra. Understanding the “3D-ness” of exoplanet atmospheres is crucial to make reliable inferences about their chemical composition, and to fully leverage the superior information content of modern telescope data. An outline of this thesis is provided below.

In **Chapter 2**, we introduce various tools for modelling and observing exoplanet atmospheres at high resolution. The main workhorse of this thesis is gCMCRT, a radiative-transfer code that can compute spectra for any planet atmosphere, while accounting for 3D variations in temperature, chemistry, and cloud coverage, as well as Doppler shifts caused by the planet’s rotation and 3D wind profile. We present the relevant equations behind the transmission and emission modes of gCMCRT and we highlight the author’s contributions to the code. Additionally, we discuss key concepts such as the cross-correlation technique and K_p - V_{sys} maps.

In **Chapter 3**, we provide a literature review of 3D effects in the atmospheres UHJs. We begin by discussing high-resolution observations that have revealed signs of “3D-ness”, and we group these into four categories. Next, we highlight some 3D modelling studies that have simulated high-resolution spectra based on outputs of global circulation models (GCMs). We summarise the lessons learned from these studies at the end of the chapter.

In **Chapter 4** (Wardenier et al. 2021), we model the phase-dependent iron absorption signal of the UHJ WASP-76b, using outputs of the SPARC/MITgcm. We model separate transmission spectra for different limb sectors, to assess how variations in temperature, chemistry, and line-of-sight velocity *across the limb* impact the overall absorption signal of the planet. Furthermore, we investigate the effect of limb asymmetries (i.e., differences between the eastern and western parts of the planet) and we compare our models to the iron signal of WASP-76b that was observed by VLT/ESPRESSO.

In **Chapter 5** (Wardenier et al. 2022), we delve into the concept of opening angles. In transmission spectroscopy, the opening angle of a planet quantifies how much “depth information” its spectrum contains (i.e., what swath of the atmosphere is probed along the line of sight). We derive a new formula for the opening angle and we use gCMCRT to compute opening angles for a grid of planets with different radii and equilibrium temperatures. Finally, we discuss the implications of our work in the context of observing UHJs.

Chapter 6 (Wardenier et al. 2023, submitted) can be seen as a follow-up to Chapter 4. We simulate the transmission spectra of different WASP-76b models in the optical and the infrared. We explore the Doppler signatures of five chemical species: Fe, TiO, CO, H₂O, and OH. Because all these species have a unique spatial distribution across the planet, they produce different absorption signals that contain complementary information about the 3D structure of the atmosphere.

Chapter 7 presents a thesis summary and some avenues for future research.

Bibliography

Alonso-Floriano F. J., et al., 2019, *A&A*, 629, A110
 Arcangeli J., et al., 2018, *ApJ*, 855, L30
 Arcangeli J., et al., 2019, *A&A*, 625, A136
 Azevedo Silva T., et al., 2022, *A&A*, 666, L10

- Batalha N. M., et al., 2013, *ApJS*, 204, 24
- Batygin K., Bodenheimer P. H., Laughlin G. P., 2016, *ApJ*, 829, 114
- Beleznay M., Kunimoto M., 2022, *MNRAS*, 516, 75
- Bell T. J., Cowan N. B., 2018, *ApJ*, 857, L20
- Bello-Arufe A., Cabot S. H. C., Mendonça J. M., Buchhave L. A., Rathcke A. D., 2022, *AJ*, 163, 96
- Beltz H., Rauscher E., Kempton E. M. R., Malsky I., Ochs G., Arora M., Savel A., 2022, *AJ*, 164, 140
- Ben-Yami M., Madhusudhan N., Cabot S. H. C., Constantinou S., Piette A., Gandhi S., Welbanks L., 2020, Technical report, Neutral Cr and V in the atmosphere of ultra hot jupiter WASP-121 b, www.hsc-chemistry.com. (arXiv:2006.05995v1), www.hsc-chemistry.com
- Bernstein R., Shectman S. A., Gunnels S. M., Mochnicki S., Athey A. E., 2003, in Iye M., Moorwood A. F. M., eds, Vol. 4841, Instrument Design and Performance for Optical/Infrared Ground-based Telescopes. SPIE, p. 1694, doi:10.1117/12.461502, <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.461502>
- Birkby J. L., 2018, arXiv e-prints, p. arXiv:1806.04617
- Bodenheimer P., Hubickyj O., Lissauer J. J., 2000, *Icarus*, 143, 2
- Borsa F., Fossati L., Koskinen T., Young M. E., Shulyak D., 2021a, *Nature Astronomy*, 6, 226
- Borsa F., et al., 2021b, *A&A*, 645, A24
- Borsa F., et al., 2022, *A&A*, 663, A141
- Borsato N. W., Hoeijmakers H., Prinoth B., Thorsbro B., Forsberg R., Kitzmann D., Jones K., Heng K., 2023, arXiv e-prints, p. arXiv:2304.04285
- Borucki W. J., et al., 2011, *ApJ*, 736, 19
- Brogi M., Snellen I. A., De Kok R. J., Albrecht S., Birkby J., De Mooij E. J., 2012, *Nature*, 486, 502
- Brogi M., de Kok R. J., Albrecht S., Snellen I. A. G., Birkby J. L., Schwarz H., 2016, *ApJ*, 817, 106
- Brogi M., et al., 2023, *AJ*, 165, 91
- Butters O. W., et al., 2010, *A&A*, 520, L10
- Cabot S. H. C., Madhusudhan N., Welbanks L., Piette A., Gandhi S., 2020, *MNRAS*, 494, 363
- Caldas A., Leconte J., Selsis F., Waldmann I. P., Bordé P., Rocchetto M., Charnay B., 2019, *A&A*, 623, A161
- Casasayas-Barris N., et al., 2018, *A&A*, 616, A151
- Casasayas-Barris N., et al., 2019, *A&A*, 628, A9
- Cauley P. W., Shkolnik E. L., Ilyin I., Strassmeier K. G., Redfield S., Jensen A., 2019, *AJ*, 157, 69
- Chene A.-N., et al., 2014, in Navarro R., Cunningham C. R., Barto A. A., eds, Vol. 9151, Advances in Optical and Mechanical Technologies for Telescopes and Instrumentation. SPIE, p. 915147, doi:10.1117/12.2057417, <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.2057417>
- Chubb K. L., Min M., 2022, *A&A*, 665, A2
- Cont D., et al., 2021, *A&A*, 651, A33
- Cont D., et al., 2022a, *A&A*, 657, L2
- Cont D., et al., 2022b, *A&A*, 668, A53
- Cosentino R., et al., 2014, in Ramsay S. K., McLean I. S., Takami H., eds, Vol. 9147, Ground-based and Airborne Instrumentation for Astronomy V. SPIE, p. 91478C, doi:10.1117/12.2055813, <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.2055813>
- Coulombe L.-P., et al., 2023, arXiv e-prints, p. arXiv:2301.08192
- Crause L. A., et al., 2014, in Ramsay S. K., McLean I. S., Takami H., eds, Vol. 9147, Ground-based and Airborne Instrumentation for Astronomy V. SPIE, p. 91476T, doi:10.1117/12.2055635, <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.2055635>
- Deeg H. J., Alonso R., 2018, Transit Photometry as an Exoplanet Discovery Method. Springer International Publishing, Cham, pp 1–25, doi:10.1007/978-3-319-30648-3_117-1, https://doi.org/10.1007/978-3-319-30648-3_117-1
- Dekker H., D’Odorico S., Kaufer A., Delabre B., Kotzlowski H., 2000, in Optical and IR Telescope Instrumentation and Detectors. SPIE, p. 534, doi:10.1117/12.395512, <https://ui.adsabs.harvard.edu/abs/2000SPIE.4008..534D/abstract>
- Donati J. F., Donati F. J., 2003, *ASPC*, 307, 41
- Ehrenreich D., et al., 2020, *Nature*, pp 1–7
- Fabrycky D., Tremaine S., 2007, *ApJ*, 669, 1298
- Falco A., Zingales T., Pluriel W., Leconte J., 2022, *A&A*, 658, A41
- Feinstein A. D., et al., 2023, *Nature*, 614, 670
- Feng Y. K., Line M. R., Fortney J. J., Stevenson K. B., Bean J., Kreidberg L., Parmentier V., 2016, *ApJ*, 829, 52

- Fischer D. A., Howard A. W., Laughlin G. P., Macintosh B., Mahadevan S., Sahlmann J., Yee J. C., 2014, in Beuther H., Klessen R. S., Dullemond C. P., Henning T., eds, *Protostars and Planets VI*. pp 715–737 ([arXiv:1505.06869](https://arxiv.org/abs/1505.06869)), doi:10.2458/azu'uapress'9780816531240-ch031
- Fischer D., et al., 2017, *AAS*, 229, 126.04
- Flowers E., Brogi M., Rauscher E., Kempton E. M.-R., Chiavassa A., 2019, *AJ*, 157, 209
- Follert R., et al., 2018, in Takami H., Evans C. J., Simard L., eds, Vol. 10702, *Ground-based and Airborne Instrumentation for Astronomy VII*. SPIE, p. 13, doi:10.1117/12.2314150, <https://spiedigitallibrary.org/conference-proceedings-of-spie/10702/2314150/CRIRES-on-its-way-to-VLT-Conference-Presentation/10.1117/12.2314150.full>
- Fortney J. J., Dawson R. I., Komacek T. D., 2021, *Journal of Geophysical Research (Planets)*, 126, e06629
- Gandhi S., Kesseli A., Snellen I., Brogi M., Wardenier J. P., Parmentier V., Welbanks L., Savel A. B., 2022, *MNRAS*, 515, 749
- Gibson N. P., et al., 2020, *MNRAS*, 493, 2215
- Gilbert J., et al., 2018, in Takami H., Evans C. J., Simard L., eds, Vol. 10702, *Ground-based and Airborne Instrumentation for Astronomy VII*. SPIE, p. 34, doi:10.1117/12.2312399, <https://www.spiedigitallibrary.org/conference-proceedings-of-spie/10702/2312399/Veloce-Rosso-Australias-new-precision-radial-velocity-spectrograph/10.1117/12.2312399.full>
- Hall R. D., Thompson S. J., Handley W., Queloz D., 2018, *MNRAS*, 479, 2968
- Hammond M., Lewis N. T., 2021, *Proceedings of the National Academy of Science*, 118, e2022705118
- Heller R., 2019, *A&A*, 628, A42
- Helling C., et al., 2019, *A&A*, 631, A79
- Helling C., et al., 2021, *A&A*, 649, A44
- Hoeijmakers H. J., de Kok R. J., Snellen I. A. G., Brogi M., Birkby J. L., Schwarz H., 2015, *A&A*, 575, A20
- Hoeijmakers H. J., et al., 2018, *Nature*, 560, 453
- Hoeijmakers H. J., et al., 2019, *A&A*, 627, A165
- Hoeijmakers H. J., et al., 2020, *A&A*, 641, A120
- Huang C. X., et al., 2018, *arXiv e-prints*, p. arXiv:1807.11129
- Jensen A. G., Redfield S., Endl M., Cochran W. D., Koesterke L., Barman T., 2012, *ApJ*, 751, 86
- Kasper D., et al., 2023, *AJ*, 165, 7
- Kesseli A. Y., Snellen I. A. G., Casasayas-Barris N., Mollière P., Sánchez-López A., 2022, *AJ*, 163, 107
- Kitzmann D., et al., 2018, *ApJ*, 863, 183
- Koch D. G., et al., 2010, *ApJ*, 713, L79
- Komacek T. D., Showman A. P., 2016, *ApJ*, 821, 16
- Komacek T. D., Tan X., 2018, *Research Notes of the AAS*, 2, 36
- Komacek T. D., Showman A. P., Tan X., 2017, *ApJ*, 835
- Komacek T. D., Tan X., Gao P., Lee E. K. H., 2022, *ApJ*, 934, 79
- Kondo S., et al., 2015, *arXiv e-prints*, p. arXiv:1501.03403
- Kotani T., et al., 2018, in SPIE. SPIE-Intl Soc Optical Eng, p. 37, doi:10.1117/12.2311836, <https://ui.adsabs.harvard.edu/abs/2018SPIE10702E..11K/abstract>
- Kozai Y., 1962, *AJ*, 67, 591
- Lacy B. I., Burrows A., 2020, *ApJ*, 905, 131
- Landman R., Sánchez-López A., Mollière P., Kesseli A. Y., Louca A. J., Snellen I. A. G., 2021, *A&A*, 656, A119
- Levine S., et al., 2018, in Takami H., Evans C. J., Simard L., eds, Vol. 10702, *Ground-based and Airborne Instrumentation for Astronomy VII*. SPIE, p. 26, doi:10.1117/12.2312345, <https://www.spiedigitallibrary.org/conference-proceedings-of-spie/10702/2312345/IGRINS-at-the-Discovery-Channel-telescope-and-Gemini-South/10.1117/12.2312345.full>
- Lidov M. L., 1962, *Planet. Space Sci.*, 9, 719
- Lin D. N. C., Bodenheimer P., Richardson D. C., 1996, *Nature*, 380, 606
- Line M. R., et al., 2021, *Nature*, 598, 580
- Lothringer J. D., Rustamkulov Z., Sing D. K., Gibson N. P., Wilson J., Schlaufman K. C., 2021, *ApJ*, 914, 12
- Louden T., Wheatley P. J., 2015, *ApJ*, 814, 1
- MacDonald R. J., Lewis N. K., 2022, *ApJ*, 929, 20
- Madhusudhan N., Knutson H., Fortney J. J., Barman T., 2014, in , *Protostars and Planets VI*. University of Arizona Press ([arXiv:1402.1169](https://arxiv.org/abs/1402.1169)), doi:10.2458/azu'uapress'9780816531240-ch032, <http://arxiv.org/abs/1402.1169>, http://dx.doi.org/10.2458/azu_uapress{ }9780816531240-ch032http://muse.jhu.edu/books/9780816598762/9780816598762-40.pdf

- Mandel K., Agol E., 2002, *ApJ*, **580**, L171
- Mayor M., Queloz D., 1995, *Nature*, **378**, 355
- Mayor M., et al., 2011, *arXiv e-prints*, p. [arXiv:1109.2497](https://arxiv.org/abs/1109.2497)
- McCarthy D. W., Burge J. H., Angel J. R. P., Ge J., Sarlot R. J., Fitz-Patrick B. C., Hinz J. L., 1998, in Fowler A. M., ed., *Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series Vol. 3354, Infrared Astronomical Instrumentation*. pp 750–754, doi:[10.1117/12.317340](https://doi.org/10.1117/12.317340)
- McLean I. S., et al., 1998, in *Infrared Astronomical Instrumentation*. SPIE, p. 566, doi:[10.1117/12.317283](https://doi.org/10.1117/12.317283), <https://ui.adsabs.harvard.edu/abs/1998SPIE.3354..566M/abstract>
- Merritt S. R., et al., 2021, *MNRAS*, **506**, 3853
- Mikal-Evans T., et al., 2022, *Nature Astronomy*, **6**, 471
- Murray-Clay R. A., Chiang E. I., Murray N., 2009, *ApJ*, **693**, 23
- Nixon M. C., Madhusudhan N., 2022, *ApJ*, **935**, 73
- Noguchi K., et al., 2002, *PASJ*, **54**, 855
- Nortmann L., et al., 2018, *Science*, **362**, 1388
- Nugroho S. K., Kawahara H., Masuda K., Hirano T., Kotani T., Tajitsu A., 2017, *AJ*, **154**, 221
- Nugroho S. K., Gibson N. P., De Mooij E. J. W., Herman M. K., Watson C. A., Kawahara H., Merritt S., 2020, Technical report, *Detection of Fe i Emission in the Day-side Spectrum of WASP-33b **. ([arXiv:2007.05508v1](https://arxiv.org/abs/2007.05508v1))
- Nugroho S. K., et al., 2021, *ApJ*, **910**, L9
- Öberg K. I., Murray-Clay R., Bergin E. A., 2011, *ApJ*, **743**, L16
- Oliva E., et al., 2012, in McLean I. S., Ramsay S. K., Takami H., eds, Vol. 8446, *Ground-based and Airborne Instrumentation for Astronomy IV*. SPIE, p. 84463T, doi:[10.1117/12.925274](https://doi.org/10.1117/12.925274), <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.925274>
- Parmentier V., et al., 2018, *A&A*, **617**
- Parmentier V., Showman A. P., Fortney J. J., 2021, *MNRAS*, **501**, 78
- Pepe F., et al., 2000, in Iye M., Moorwood A. F. M., eds, Vol. 4008, *Optical and IR Telescope Instrumentation and Detectors*. SPIE, p. 582, doi:[10.1117/12.395516](https://doi.org/10.1117/12.395516), <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.395516>
- Pepe F. A., et al., 2010, in *Ground-based and Airborne Instrumentation for Astronomy III*. SPIE, p. 77350F, doi:[10.1117/12.857122](https://doi.org/10.1117/12.857122), <https://ui.adsabs.harvard.edu/abs/2010SPIE.7735E..0FP/abstract>
- Pepper J., et al., 2007, *PASP*, **119**, 923
- Pino L., et al., 2020, *ApJ*, **894**, L27
- Pluriel W., 2023, *Remote Sensing*, **15**
- Pluriel W., Zingales T., Leconte J., Parmentier V., 2020, *A&A*, **636**, A66
- Pluriel W., Leconte J., Parmentier V., Zingales T., Falco A., Selsis F., Bordé P., 2022, *A&A*, **658**, A42
- Pollacco D. L., et al., 2006, *PASP*, **118**, 1407
- Prinoth B., et al., 2022, *Nature Astronomy*, **6**, 449
- Quirrenbach A., Consortium C., Quirrenbach A., Consortium C., 2016, *cosp*, **41**, E1.21
- Rasio F. A., Tout C. A., Lubow S. H., Livio M., 1996, *ApJ*, **470**, 1187
- Rayner J., et al., 2016, in Evans C. J., Simard L., Takami H., eds, Vol. 9908, *Ground-based and Airborne Instrumentation for Astronomy VI*. SPIE, p. 990884, doi:[10.1117/12.2232064](https://doi.org/10.1117/12.2232064), <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.2232064>
- Ricker G. R., et al., 2015, *Journal of Astronomical Telescopes, Instruments, and Systems*, **1**, 014003
- Ridden-Harper de Mooij E., Jayawardhana R., Gibson N., Karjalainen R., Karjalainen M., 2023, *arXiv e-prints*, p. [arXiv:2304.03248](https://arxiv.org/abs/2304.03248)
- Roth A., Drummond B., Hébrard E., Tremblin P., Goyal J., Mayne N., 2021, *MNRAS*, **505**, 4515
- Sánchez-López A., Landman R., Mollière P., Casasayas-Barris N., Kesseli A. Y., Snellen I. A. G., 2022, *A&A*, **661**, A78
- Savel A. B., et al., 2022, *ApJ*, **926**, 85
- Schwarz H., Ginski C., De Kok R. J., Snellen I. A. G., Brogi M., Birkby J. L., 2016, *A&A*, **593**
- Seidel J. V., et al., 2019, *A&A*, **623**, A166
- Seidel J. V., Ehrenreich D., Pino L., Bourrier V., Lavie B., Allart R., Wyttenbach A., Lovis C., 2020, *A&A*, **633**, A86
- Seifahrt A., Stürmer J., Bean J. L., Schwab C., 2018, in Takami H., Evans C. J., Simard L., eds, Vol. 10702, *Ground-based and Airborne Instrumentation for Astronomy VII*. SPIE, p. 232, doi:[10.1117/12.2312936](https://doi.org/10.1117/12.2312936), <https://www.spiedigitallibrary.org/conference-proceedings-of-spie/10702/2312936/MAROON-X--a-radial-velocity-spectrograph-for-the-Gemini/10.1117/12.2312936.full>

- Sheinis A. I., 2016, in Evans C. J., Simard L., Takami H., eds, Vol. 9908, Ground-based and Airborne Instrumentation for Astronomy VI. SPIE, p. 99081C, doi:10.1117/12.2234334, <http://proceedings.spiedigitallibrary.org/proceeding.aspx?doi=10.1117/12.2234334>
- Showman A. P., Guillot T., 2002, *A&A*, 385, 166
- Showman A. P., Cooper C. S., Fortney J. J., Marley M. S., 2008, *ApJ*, 682, 559
- Sindel J. P., Ehrenreich D., Hoeijmakers J., 2018, Technical report, The transmission spectrum of WASP-121b in high resolution with HARPS
- Snellen I. A. G., De Kok R. J., De Mooij E. J. W., Albrecht S., 2010, *Nature*, 465, 1049
- Snellen I. A., Brandl B. R., De Kok R. J., Brogi M., Birkby J., Schwarz H., 2014, *Nature*, 508, 63
- Snellen I., et al., 2015, *A&A*, 576, A59
- Stangret M., Casasayas-Barris N., Pallé E., Yan F., Sánchez-López A., López-Puertas M., 2020, *A&A*, 638, A26
- Stevens D. J., Gaudi B. S., 2013, *PASP*, 125, 933
- Strassmeier K. G., et al., 2015, *Astronomische Nachrichten*, 336, 324
- Tabernero H. M., et al., 2021, *A&A*, 646, A158
- Talens G. J. J., Spronck J. F. P., Lesage A. L., Otten G. P. P. L., Stuik R., Pollacco D., Snellen I. A. G., 2017, *A&A*, 601, A11
- Tan X., Komacek T. D., 2019, *ApJ*, 886, 26
- Taylor J., Parmentier V., Irwin P. G. J., Aigrain S., Lee E. K. H., Krissansen-Totton J., 2020, *MNRAS*, 493, 4342
- Tennyson J., Yurchenko S. N., 2012, *Monthly Notices of the Royal Astronomical Society*, 425, 21
- Thibault S., et al., 2012, in Ground-based and Airborne Instrumentation for Astronomy IV. SPIE, p. 844630, doi:10.1117/12.926697, <https://ui.adsabs.harvard.edu/abs/2012SPIE.8446E..30T/abstract>
- Thompson S. J., et al., 2016, in Evans C. J., Simard L., Takami H., eds, Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series Vol. 9908, Ground-based and Airborne Instrumentation for Astronomy VI. p. 99086F (arXiv:1608.04611), doi:10.1117/12.2232111
- Tull R. G., 1998, in Optical Astronomical Instrumentation. SPIE, pp 387–398, doi:10.1117/12.316774, <https://ui.adsabs.harvard.edu/abs/1998SPIE.3355..387T/abstract>
- Turner J. D., et al., 2020, *ApJLetters*, 888, L13
- Van Sluijs L., et al., 2022, arXiv e-prints, p. arXiv:2203.13234
- Vogt S. S., et al., 1994, in Crawford D. L., Craine E. R., eds, Vol. 2198, Instrumentation in Astronomy VIII. SPIE, pp 362–375, doi:10.1117/12.176725, <https://ui.adsabs.harvard.edu/abs/1994SPIE.2198..362V/abstract> <http://proceedings.spiedigitallibrary.org/proceeding.aspx?articleid=959834>
- Wakeford H. R., Visscher C., Lewis N. K., Kataria T., Marley M. S., Fortney J. J., Mandell A. M., 2017, *MNRAS*, 464, 4247
- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, *MNRAS*, 506, 1258
- Wardenier J. P., Parmentier V., Lee E. K. H., 2022, *MNRAS*, 510, 620
- Wildi F., et al., 2017, in Shaklan S., ed., Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series Vol. 10400, Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series. p. 1040018, doi:10.1117/12.2275660
- Wright J. T., 2018, Radial Velocities as an Exoplanet Discovery Method. Springer International Publishing, Cham, pp 619–631, doi:10.1007/978-3-319-55333-7_4, https://doi.org/10.1007/978-3-319-55333-7_4
- Wright J. T., Marcy G. W., Howard A. W., Johnson J. A., Morton T. D., Fischer D. A., 2012, *ApJ*, 753, 160
- Yan F., Henning T., 2018, *Nature Astronomy*, 2, 714
- Yan F., et al., 2019, *A&A*, 632, A69
- Yan F., et al., 2020, *A&A*, 640, L5
- Yan F., et al., 2021, *A&A*, 645, A22
- Yan F., et al., 2022, *A&A*, 661, L6
- Yan F., et al., 2023, arXiv e-prints, p. arXiv:2302.08736
- de Regt S., Kesseli A. Y., Snellen I. A. G., Merritt S. R., Chubb K. L., 2022, *A&A*, 661, A109

Chapter 2

Methods for modelling and observing exoplanet atmospheres at high spectral resolution

The material in this chapter is partly based on [Wardenier et al. \(2021\)](#):

– Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, MNRAS, 506, 1258

Abstract – *In this chapter, we present a new 3D framework for modelling phase-dependent transmission and emission spectra of exoplanets at high spectral resolution. The framework relies on a GPU-optimised Monte-Carlo radiative transfer code, gCMCRT, to post-process the outputs of the SPARC/MITgcm global circulation model. gCMCRT can compute spectra for an arbitrary planet atmosphere, accounting for 3D variations in temperature, chemistry, and cloud coverage, as well as Doppler shifts caused by the planet’s rotation and 3D wind profile. This allows to correctly model the countless number of spectral lines that can be observed with ground-based high-resolution spectrographs. In what follows, we will discuss the essential equations behind the transmission and emission modes of gCMCRT. Additionally, we will show how the framework accounts for Doppler shifts induced by nonzero line-of-sight velocities in the atmosphere. We also benchmark the high-resolution version of gCMCRT against a 1D radiative transfer code that uses the same opacities. Finally, we discuss some other ubiquitous concepts from high-resolution spectroscopy, such as singular-value decomposition (SVD), the cross-correlation function (CCF), and K_p – V_{sys} maps.*

2.1 The SPARC/MITgcm

In this section, we will provide a short qualitative description of the SPARC/MITgcm ([Showman et al. 2009](#)), which was used to generate the 3D atmospheric models used in this thesis (see Fig. 2.1). The SPARC/MITgcm comprises two components: (i) a dynamical core, taken from the MITgcm ([Adcroft et al. 2004](#)), and (ii) a plane-parallel radiative-transfer module developed by [Marley & McKay \(1999\)](#). Starting from a set of initial conditions, the atmosphere evolves in an iterative fashion, whereby the output of the dynamical core serves as an input for the radiative-transfer module, and vice versa. Based on the wind field $\vec{v}$ and the temperatures T from the previous iteration, as well as a heating flux ∇F obtained from the radiative-transfer, the dynamical core solves the primitive equations (e.g., [Lions et al. 1992](#); [Vallis 2017](#)) to obtain new values for $\vec{v}$ and T . These are then passed to the radiative-transfer module to calculate new upward and downward fluxes, and update the heating rate.

Radiative transfer in the SPARC/MITgcm is performed across 11 wavelength bins ([Kataria et al. 2015](#)) between 0.26 and 325 microns¹, and relies on the correlated- k method ([Goody et al. 1989](#); [Fu & Liou 1992](#); [Mollière et al. 2015](#)). In the correlated- k method, one builds a cumulative distribution of the opacity values (at millions of wavelength points) in each

¹Radiative transfer with wavelength-dependent opacities is known as *non-grey* radiative transfer. Other GCMs (e.g., [Rauscher & Menou 2012](#)) employ a *double-grey* scheme, whereby two opacity functions $\kappa_{\text{vis}}(P, T)$ and $\kappa_{\text{IR}}(P, T)$ (with P pressure and T temperature) are assigned to the optical and the infrared, respectively.

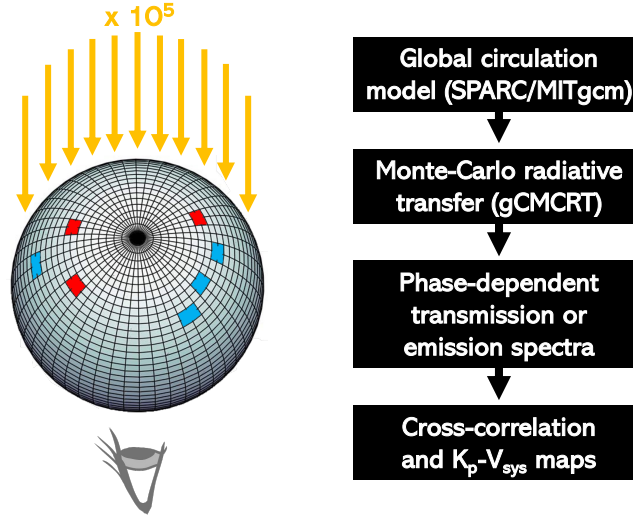


Figure 2.1: Schematic overview of the framework used in this thesis to compute transmission and emission spectra of 3D exoplanet atmospheres. The image on the left visualises the transmission calculations performed by gCMCRT (see Section 2.2). A beam of photon packets strike the atmosphere of the planet, defined on a spherical grid. Each atmospheric cell has its own temperature, composition, and wind vectors. In each cell, opacities are blueshifted or redshifted, depending on the local line-of-sight velocity.

bin. During the radiative transfer, one then samples this distribution at a couple of Gaussian quadrature points (8 in this work) to obtain an accurate approximation of the absorption, rather than having to evaluate it at many wavelengths. This dramatically speeds up the calculations. The correlated- k method is accurate as long as the opacity distribution in a bin does not strongly vary with height in an atmospheric column (hence the name *correlated-k*). In the SPARC/MITgcm, separate radiative transfer calculations are carried out for (i) incident stellar light and (ii) thermal emission by the planet. We refer to [Showman et al. \(2009\)](#) for further details.

It is worth mentioning three characteristic timescales associated with GCM calculations: the radiative timescale τ_{rad} , the drag timescale τ_{drag} , and the wave timescale τ_{wave} (e.g., [Komacek & Showman 2016](#); [Parmentier & Crossfield 2018](#)). τ_{rad} is the typical time that passes before an air parcel has lost a significant amount of its heat through radiation. In the GCM, its value results from the non-grey (i.e., wavelength-dependent) radiative transfer ([Showman et al. 2015](#)). In a similar spirit, τ_{drag} is the time it takes for the air parcel to lose a substantial portion of kinetic energy. The drag timescale encapsulates a variety of physical mechanisms that can cause atmospheric drag, such as turbulent mixing ([Li & Goodman 2010](#)), Lorentz-force braking of ionised winds in the planet’s magnetic field ([Perna et al. 2010a](#)), and Ohmic dissipation ([Perna et al. 2010b](#)). τ_{drag} is a tunable parameter in the GCM. It can be included in an additional “Rayleigh drag” term $-\vec{v}/\tau_{\text{drag}}$ in the momentum equation solved by the dynamical core. This approach assumes that the drag force is uniform across the whole planet atmosphere.

Finally, τ_{wave} is the time in which a gravity wave travels a distance similar to the planet radius. In the context of (ultra-)hot Jupiters, the value of the wave timescale compared to the radiative and the drag timescales determines what dynamic regime the atmosphere falls in. If $\tau_{\text{rad}}, \tau_{\text{drag}} \gtrsim \tau_{\text{wave}}$, the atmosphere will develop a superrotating jet and heat transport will be relatively efficient. On the other hand, if $\tau_{\text{rad}}, \tau_{\text{drag}} < \tau_{\text{wave}}$, the dynamics will be dominated by a day-to-night flow.

2.2 Monte-Carlo radiative transfer with gCMCRT

In this section, we will describe the relevant aspects of gCMCRT² (Lee et al. 2022, incl. Wardenier). gCMCRT is a 3D Monte-Carlo radiative transfer code (written in Fortran) that is GPU-compatible. This means that the code can take full advantage of the parallel architecture of a GPU, which comprises hundreds to thousands of individual cores (processing units). Hence, a large number of radiative-transfer calculations can be performed simultaneously, making gCMCRT much faster (ca. 100×) than its precursor, CMCRT (Lee et al. 2017, 2019), which ran on CPUs. In Lee et al. (2019), the low-resolution version of CMCRT was benchmarked against several other (1D) radiative transfer codes. In Wardenier et al. (2021), we added *high-resolution* functionalities to CMCRT, which were subsequently incorporated into the first release of gCMCRT. Specifically, the author of this thesis made the following contributions:

- Writing a module to read high-resolution opacities that are also used by the CHIMERA 1D radiative transfer code (see Section 2.2.5).
- Implementing the equation for Doppler shifts into the radiative transfer, such that the opacities in each atmospheric cell are shifted according to their local line-of-sight velocity (see Sections 2.2.1 and 2.2.3).
- Adapting the code such that it can produce transmission spectra associated with specific limb sectors (see Section 2.2.2), as well as with different orbital phases during a *single* run. With the current architecture, opacities only have to be read once, regardless of the number of phases at which the spectra are being simulated. The same holds for the emission mode.
- Benchmarking the transmission and emission modes of gCMCRT against outputs from CHIMERA (see Section 2.2.5).
- Writing a function that allows to construct absorption regions (see Chapters 5 and 6) that indicate what parts of the atmosphere are probed at a given orbital phase, at a given wavelength.
- Developing a Python framework that dynamically handles job submissions to a computer cluster, based on the number of available cores/nodes and their performance. The framework automatically generates input files for gCMCRT and allows the user to compute spectra across a parameter space (e.g., different wavelength bands, resolutions, orbital phases, atmospheric structures, Doppler shifts on/off, etc.) with little effort.

In general, Monte-Carlo radiative transfer (Hood et al. 2008; Whitney 2011; Steinacker et al. 2013; Stolker et al. 2017; Lee et al. 2017, 2019; Noebauer & Sim 2019) relies on *photon packets*, which perform a random walk throughout a 3D medium of interest. Every time the packet undergoes an interaction, its attributes (e.g., luminosity, direction, polarisation) are updated, until it escapes from the medium. To avoid over-complicating our model and build physical understanding, we do not explicitly treat multiple-scattering in this thesis, but we leave it for future work. In transmission, scattering can be adequately accounted for

²gCMCRT stands for GPU Cloudy Monte-Carlo Radiative Transfer. The code is publicly available from github.com/ELeeAstro/gCMCRT

by including an extra absorption term, as scattering causes photons to *depart* from the line of sight and not contribute to the flux (such that the effect of a scattering particle is the same as that of an absorbing particle). In emission, not treating scattering is justified when considering a wavelength region in which Rayleigh scattering is negligible. Effectively, we use gCMCRT as a *randomised extinction chord algorithm* (Lee et al. 2019), in which the propagation direction of the photon packets does not change after their initialisation. It should be noted that this method is probabilistic and that the spectrum converges to the true solution with an increasing number of photon packets.

In the following paragraphs, we will provide the essential equations behind both the transmission and the emission modes of gCMCRT.

2.2.1 Transmission spectroscopy

The transmission equation

As a planet passes in front of its host star, a fraction of the stellar light interacts with the planetary atmosphere, where it falls prey to absorption and scattering. Because the opacity κ of the atmospheric constituents is wavelength-dependent, the apparent radius $R_p(\lambda)$ of the planet also varies with wavelength. Measuring $R_p(\lambda)$ at different wavelengths gives rise to the planet’s transmission spectrum, which is commonly expressed as a depth:

$$\delta(\lambda) = \frac{F_{\text{out}}(\lambda) - F_{\text{in}}(\lambda)}{F_{\text{out}}(\lambda)} = \frac{R_p^2(\lambda)}{R_\star^2}, \quad (2.1)$$

where F_{out} and F_{in} are the received out-of-transit and in-transit stellar fluxes, respectively. Furthermore, $R_\star$ is the stellar radius. Equation 2.1 can be expanded to obtain

$$\delta(\lambda) = \frac{1}{\pi R_\star^2} \left[\pi R_0^2 + \int_0^{2\pi} \int_0^{z_{\text{max}}} (R_0 + z) (1 - e^{-\tau(\lambda, z, \Theta)}) dz d\Theta \right], \quad (2.2)$$

where R_0 denotes the radius of the planet at the (optically thick) “bottom” of the atmosphere, while the atmosphere itself extends from R_0 to $R_0 + z_{\text{max}}$. The expression contained in the integral is the product of the impact parameter $b = R_0 + z$ and the transmission, where τ denotes the optical depth as a function of wavelength, altitude z , and impact angle Θ .

If we assume that the temperature and the composition of the atmosphere only vary with altitude, it holds that $\tau = \tau(\lambda, z)$. In this one-dimensional case, we can eliminate Θ from Equation 2.2, which yields (e.g., Tinetti et al. 2012)

$$\delta(\lambda) = \frac{1}{R_\star^2} \left[R_0^2 + 2 \int_0^{z_{\text{max}}} (R_0 + z) (1 - e^{-\tau(\lambda, z)}) dz \right]. \quad (2.3)$$

From these expressions, it can be readily seen that $\delta = R_0^2/R_\star^2$ for a completely transparent atmosphere ($\tau = 0$). On the other hand, $\delta = (R_p + z_{\text{max}})^2/R_\star^2$ for an atmosphere that is fully opaque ($\tau \rightarrow \infty$). In the rest of this thesis, however, we will consider a 3D planetary structure and we will need to numerically integrate Equation 2.2 as a function of z and Θ .

Computing transmission spectra with gCMCRT

To compute $R_p(\lambda)$, gCMCRT initialises n photon packets for every wavelength in the spectral window of interest ($n = 10^5$ throughout this work). Each photon packet is assigned

a random impact parameter $b \in (R_0, R_0 + z_{\max})$ and impact angle $\Theta \in [0, 2\pi)$, in such a way that the atmospheric annulus is uniformly sampled. For each photon packet, gCMCRT then evaluates the optical depth $\tau(\lambda, b, \Theta)$ along the corresponding transit chord in a 3D spherical geometry. The optical depth is given by

$$\tau(\lambda, b, \Theta) = \sum_{i=1}^{N_{\text{cells}}} \rho_i \tilde{\kappa}_i(\lambda, v_{\text{LOS}}) \Delta x_i, \quad (2.4)$$

where $\tilde{\kappa}_i$ is the opacity (with units cm^2/g) of the i -th atmospheric cell, ρ_i the density, and Δx_i the distance the photon packet travels through the cell. Note that in high spectral resolution, the effective opacity depends on both the wavelength of the photon packet (in the observer's frame) and the velocity v_{LOS} of the medium along the line of sight. v_{LOS} is nonzero due to (i) atmospheric dynamics (i.e. winds), (ii) the rotation of the planet, (iii) its orbital motion and (iv) the system velocity. In this work, however, we assume that all spectra are shifted to the *planetary rest frame*, where the contributions from (iii) and (iv) are zero. Given a particular atmospheric cell, the line-of-sight velocity can thus be written as (e.g., [Harada et al. 2021](#))

$$\begin{aligned} v_{\text{LOS}} = & -u \sin(\varphi + \phi) \\ & -v \cos(\varphi + \phi) \sin(\alpha) \\ & +w \cos(\varphi + \phi) \cos(\alpha) \\ & -\Omega(R_0 + z) \sin(\varphi + \phi) \cos(\alpha), \end{aligned} \quad (2.5)$$

where the first three terms represent the contribution from winds and the last term is due to the rotation of the planet. In Equation 2.5, (u, v, w) is the cell's wind vector, with u the component in the local west-to-east (zonal) direction, v the component in the local south-to-north (meridional) direction and w the component in the local nadir-to-zenith (vertical) direction. $\alpha \in [-90^\circ, 90^\circ]$, $\varphi \in [-180^\circ, 180^\circ)$ and $z \in [0, z_{\max}]$ denote the latitude, longitude and altitude of the cell, respectively. Furthermore, $\phi \in [-180^\circ, 180^\circ)$ is the orbital phase angle, which is zero at the primary transit and $\pm 180^\circ$ at the secondary eclipse. Ω denotes the planet's angular frequency (with units rad/s). In order for Equation 2.5 to hold, the planet must be tidally locked, such that the sub-stellar point is always given by $\alpha = \varphi = 0$. Also, we assume that the orbit is viewed exactly edge-on. Because Equation 2.5 is key to our modelling efforts, a derivation is provided in Section 2.2.3.

Once the line-of-sight velocity of a cell is known, $\tilde{\kappa}_i$ can be computed by evaluating the opacity function κ_i at an effective wavelength λ_{eff} to account for the associated Doppler shift:

$$\tilde{\kappa}_i(\lambda, v_{\text{LOS}}) = \kappa_i(\lambda_{\text{eff}}), \text{ with } \lambda_{\text{eff}} = \lambda \left[1 - \frac{v_{\text{LOS}}}{c} \right]. \quad (2.6)$$

From this equation, it follows that $\lambda_{\text{eff}} > \lambda$ when the medium moves towards the observer, which seems counter-intuitive. However, from the perspective of the atmospheric cell, $v_{\text{LOS}} < 0$ means that the star is moving away, so the effective wavelength seen by the medium should be redshifted relative to the wavelength seen by the observer.

Once the optical depth is computed along all n transit chords, the transit radius $R_p(\lambda)$ can be found from

$$R_p^2(\lambda) = R_0^2 + \left((R_0 + z_{\max})^2 - R_0^2 \right) \left\langle 1 - e^{-\tau} \right\rangle_{\lambda} \quad (2.7)$$

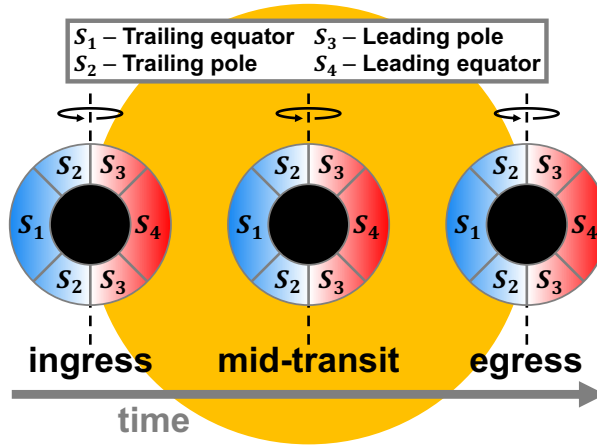


Figure 2.2: Schematic view of a planet at three stages during its transit, with the host star shown in the background. The planet's atmospheric annulus is divided into four limb sectors with equal area: the trailing equator (S_1), the trailing pole (S_2), the leading pole (S_3) and the leading equator (S_4). Because of planetary rotation, opacities along the line of sight are Doppler shifted, resulting in a blueshift on the trailing limb (S_1+S_2) and a redshift on the leading limb (S_3+S_4). Effects of winds are not visualised here.

where the angle brackets denote an average over all photon packets with wavelength λ . Equation 2.7 follows from Equation 2.3 (or 2.2) by (i) applying the mean value theorem for integrals and (ii) assuming that the photon packets are *uniformly distributed* across the atmospheric annulus.

Alternatively, we can write the above expression in terms of areas:

$$A_p(\lambda) = A_0 + A_{\text{annu}} \langle 1 - e^{-\tau} \rangle_\lambda \quad (2.8)$$

with $A_p(\lambda)$ the effective area of the planet, A_0 the projected area of the planetary interior and A_{annu} the area of the atmospheric annulus. Again, it can be readily seen that $A_p = A_0$ when the atmosphere is transparent ($\tau \rightarrow 0$), while $A_p = A_0 + A_{\text{annu}}$ when the atmosphere is completely opaque ($\tau \rightarrow \infty$).

2.2.2 Decomposing the atmosphere into limb sectors

Since the final spectrum $A_p(\lambda)$ represents an average over the entire – spatially varying – limb of the planet, it is hard to identify *how* and to what extent different parts of the atmosphere actually contribute to the overall observable. A way to alleviate this problem is to divide the atmospheric annulus into limb sectors S_i (see Figure 2.2) and to consider the contributions from each of these sectors separately.

One of the advantages of gCMCRT is that the code can compute transit spectra for any arbitrary subregion of the atmospheric annulus. These spectra can also be found through Equation 2.8, with the only addition that the average is taken over the transit chords (or, equivalently, photon packets) that cross the sector:

$$A_{p,i}(\lambda) = A_0 + A_{\text{annu}} \langle 1 - e^{-\tau} \rangle_{\lambda, S_i} \quad (2.9)$$

Since we multiply the average extinction with the total area A_{annu} of the atmospheric annulus, $A_{p,i}(\lambda)$ represents the effective planet area that would be observed if the full limb had

the same structure, composition and dynamics as sector $\mathcal{S}_i$.

Suppose we now divide the limb into N_s arbitrary, non-overlapping sectors. In this case, Equation 2.8 can be written as

$$A_p(\lambda) = \sum_{i=1}^{N_s} \beta_i \cdot \left(A_0 + A_{\text{annu}} \langle 1 - e^{-\tau} \rangle_{\lambda, \mathcal{S}_i} \right) = \sum_{i=1}^{N_s} \beta_i \cdot A_{p,i}(\lambda) \quad (2.10)$$

with β_i the fractional area of sector $\mathcal{S}_i$, such that $\sum \beta_i = 1$. This result demonstrates that the spectrum of the full limb is a weighted sum of the spectra of the individual sectors. Furthermore, when all limb sectors have the same area (as in Figure 2.2), we find that

$$A_p(\lambda) = \langle A_{p,i}(\lambda) \rangle, \quad (2.11)$$

where the angle brackets denote an average over all limb sectors.

2.2.3 Line-of-sight velocities

In this section, we will provide a derivation of Equation 2.5, which we use to calculate the line-of-sight velocity by which the opacities are shifted in the during the radiative transfer. We start by defining a local Cartesian coordinate system $\{\hat{u}, \hat{v}, \hat{w}\}$ in each atmospheric cell. As shown in Figure 2.3, $\hat{u}$ points into the local west-to-east direction, $\hat{v}$ points into the local south-to-north direction and $\hat{w}$ points upwards, perpendicular to the local surface.

In the atmospheric structure read by gCMCRT, the wind vectors are defined in the local frames of the atmospheric cells. Hence, to obtain the effective line-of-sight velocities, we must project the wind vectors onto a viewing vector $\hat{k}$, a unit vector that points towards the observer. It is most convenient to perform this projection in a coordinate system $\{\hat{x}, \hat{y}, \hat{z}\}$ that co-rotates with the planet (see Figure 2.3). Here, $\hat{x}$ and $\hat{y}$ span the orbital plane, such $\hat{x}$ always points towards the host star. In this setup, observing the planet at different phase angles or orbital inclinations is simply a matter of changing the viewing vector $\hat{k}$.

Our first step is to express the unit vectors $\{\hat{u}, \hat{v}, \hat{w}\}$ in the $\{\hat{x}, \hat{y}, \hat{z}\}$ frame:

$$\hat{u} = \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \\ 0 \end{pmatrix} \quad \hat{v} = \begin{pmatrix} -\cos(\theta) \cos(\varphi) \\ -\cos(\theta) \sin(\varphi) \\ \sin(\theta) \end{pmatrix} \quad \hat{w} = \begin{pmatrix} \sin(\theta) \cos(\varphi) \\ \sin(\theta) \sin(\varphi) \\ \cos(\theta) \end{pmatrix}, \quad (2.12)$$

where θ and φ are the spherical coordinates of the cell, as denoted in Figure 2.3. The expression for $\hat{w}$ is trivial, as it points into the radial direction. Additionally, $\hat{u}$ is always tangent to the equator, so it must be confined to the x - y plane. The expression for $\hat{v}$ is less intuitive, but can be obtained from the cross product $\hat{w} \times \hat{u}$. Additionally, we can write the viewing vector $\hat{k}$ as

$$\hat{k} = \begin{pmatrix} \sin(\theta_v) \cos(\varphi_v) \\ \sin(\theta_v) \sin(\varphi_v) \\ \cos(\theta_v) \end{pmatrix}, \quad (2.13)$$

with θ_v and φ_v the viewing angles of the observer that define the line of sight. For an edge-on orbit, $\theta_v = 90^\circ$ and the third component of $\hat{k}$ becomes zero.

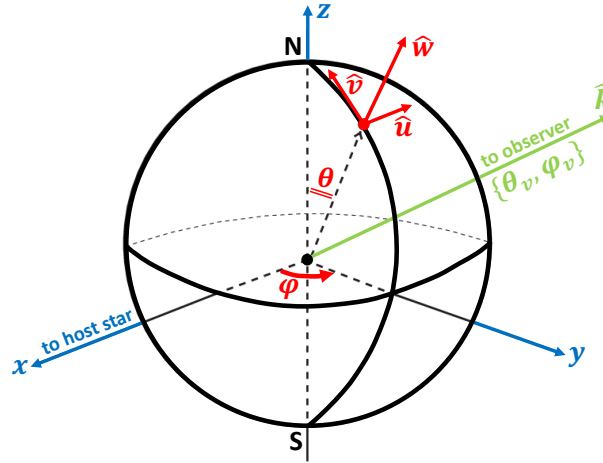


Figure 2.3: A graphic depiction of a local coordinate system $\{\hat{u}, \hat{v}, \hat{w}\}$ (in red) and the frame that co-rotates with the planet (in blue). The angle φ is measured counter-clockwise from the positive x axis, while θ is the angle between $\hat{w}$ and the z axis. The viewing vector $\hat{k}$ is a unit vector which points towards the observer and has associated angles θ_v and φ_v . N and S denote the planet's north and south pole, respectively. Image adapted from [Constantin & Johnson \(2017\)](#).

Contribution from winds

Given the wind vector (u, v, w) in a particular atmospheric cell, the effective wind speed v_{LOS} along the line of sight is given by

$$v_{\text{LOS}} = -\hat{k} \cdot (u\hat{u} + v\hat{v} + w\hat{w}), \quad (2.14)$$

where the minus sign accounts for the fact that velocities are negative when they point towards the observer. Plugging in Equations 2.12 and 2.13, and working out the inner products yields:

$$\begin{aligned} -u\hat{k} \cdot \hat{u} &= u \sin(\theta_v) \sin(\varphi - \varphi_v) \\ -v\hat{k} \cdot \hat{v} &= v \cos(\theta) \sin(\theta_v) \cos(\varphi - \varphi_v) - v \sin(\theta) \cos(\theta_v) \\ -w\hat{k} \cdot \hat{w} &= -w \sin(\theta) \sin(\theta_v) \cos(\varphi - \varphi_v) - w \cos(\theta) \cos(\theta_v). \end{aligned} \quad (2.15)$$

Combining these terms, Equation 2.14 now reads:

$$\begin{aligned} v_{\text{LOS}} &= u \sin(\theta_v) \sin(\varphi - \varphi_v) \\ &\quad + [v \cos(\theta) - w \sin(\theta)] \sin(\theta_v) \cos(\varphi - \varphi_v) \\ &\quad - [v \sin(\theta) + w \cos(\theta)] \cos(\theta_v). \end{aligned} \quad (2.16)$$

To obtain the first three terms of Equation 2.5, we need to make a number of substitutions. Firstly, $\theta_v = 90^\circ$ under the assumption of an edge-on orbit, such that the final term in Equation 2.16 drops out. Furthermore, $\varphi_v = (180^\circ - \varphi)$ and $\theta = (90^\circ - \alpha)$ allow for the line-of-sight velocity to be expressed in terms of the orbital phase angle ϕ and the cell's latitude α . Note that these relationships change when the orientation of the orbit is different.

Contribution from planetary rotation

The rotation of the planet also gives rise to a line-of-sight velocity term. This is because the $\{\hat{x}, \hat{y}, \hat{z}\}$ frame is rotating with respect to the observer. For a planet that is tidally locked, the rotation period is equal to the orbital period, with an associated angular frequency Ω (with units rad/s).

For each atmospheric cell, the velocity vector $\vec{v}$ due to rotation only points into the local $\hat{u}$ direction, perpendicular to the planetary axis. Its magnitude depends on the latitude and altitude z of the atmospheric cell:

$$\vec{v} = \Omega(R_0 + z) \sin(\theta) \hat{u}. \quad (2.17)$$

Here, R_0 is the planetary radius at the bottom of the atmosphere, such that $R_0 + z$ is the distance from the cell to the centre of the planet. Ω is positive when the $\{\hat{x}, \hat{y}, \hat{z}\}$ frame rotates counter-clockwise as seen from the positive z axis. The resulting line-of-sight velocity is

$$\begin{aligned} v_{\text{LOS}} &= -\hat{k} \cdot \vec{v} \\ &= \Omega(R_0 + z) \sin(\theta) \sin(\theta_v) [\sin(\varphi) \cos(\varphi_v) - \cos(\varphi) \sin(\varphi_v)] \\ &= \Omega(R_0 + z) \sin(\theta) \sin(\theta_v) \sin(\varphi - \varphi_v). \end{aligned} \quad (2.18)$$

By substituting $\theta_v = 90^\circ$, $\varphi_v = (180^\circ - \phi)$ and $\theta = (90^\circ - \alpha)$, we recover the final term in Equation 2.5.

2.2.4 Emission spectroscopy

Atmospheric emission

To compute the emission spectrum of an atmosphere, gCMCRT assigns a luminosity L_i (with units erg/s/cm) to every atmospheric cell i at each wavelength³. In this section we will derive an expression for this luminosity, based on the radiative-transfer equation and principles of radiative equilibrium.

Given a wavelength window $\lambda \in [\lambda_1, \lambda_2]$, a region is in (pointwise) radiative equilibrium when

$$\int_{\lambda_1}^{\lambda_2} \vec{\nabla} I_\lambda d\lambda = \vec{0} \quad (2.19)$$

at every point contained in the region (e.g., [Mihalas 1978](#)). Equation 2.19 essentially summarises that the intensity (that is, the specific intensity I_λ integrated over all wavelengths λ) may not change along any direction vector – every point in space must emit as much energy as it receives. From the equation of radiative transfer, it now follows that

$$\int_{\lambda_1}^{\lambda_2} (-\alpha_\lambda I_\lambda + j_\lambda) d\lambda = \int_{\lambda_1}^{\lambda_2} \alpha_\lambda (S_\lambda - I_\lambda) d\lambda = 0, \quad (2.20)$$

with α_λ the absorption coefficient, j_λ the emission coefficient and $S_\lambda \equiv j_\lambda / \alpha_\lambda$ the source function. Assuming that the radiation field is isotropic and that the medium is in thermal equilibrium at a temperature T , Equation 2.20 can be written as

³The correct notation would be $L_{i,\lambda}$, but we drop the dependence on wavelength for notational convenience.

$$\int_{\lambda_1}^{\lambda_2} \alpha_\lambda (B_\lambda(T) - J_\lambda) d\lambda = \rho \int_{\lambda_1}^{\lambda_2} \kappa_\lambda (B_\lambda(T) - J_\lambda) d\lambda = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda (B_\lambda(T) - J_\lambda) d\lambda = 0. \quad (2.21)$$

Here, B_λ is the black-body function and $J_\lambda \equiv \int I_\lambda d\lambda / 4\pi$ is the mean specific intensity. Furthermore, ρ is the density of the medium and $\kappa_\lambda = \alpha_\lambda / \rho$ is the opacity (with units cm^2/g). Splitting the integral yields

$$\int_{\lambda_1}^{\lambda_2} \kappa_\lambda J_\lambda d\lambda = \int_{\lambda_1}^{\lambda_2} \kappa_\lambda B_\lambda(T) d\lambda, \quad (2.22)$$

where the left-hand side can be recognised as the total intensity that is absorbed by a medium of unit mass, per unit solid angle. By the virtue of radiative equilibrium, this is also the intensity that is emitted. Hence, the luminosity L_i of an atmospheric cell at a given wavelength obeys

$$\int_{\lambda_1}^{\lambda_2} L_i d\lambda = 4\pi m_i \int_{\lambda_1}^{\lambda_2} \kappa_\lambda B_\lambda(T) d\lambda = 4\pi \rho_i V_i \int_{\lambda_1}^{\lambda_2} \kappa_\lambda B_\lambda(T) d\lambda, \quad (2.23)$$

with m_i the cell's mass, ρ_i the cell's density and V_i the cell's volume. This gives

$$L_i = 4\pi \rho_i V_i \kappa_\lambda B_\lambda(T), \quad (2.24)$$

which coincides with expressions provided in [Pinte et al. \(2006\)](#) and [Lee et al. \(2017\)](#).

The bias technique

In pure (*non-biased*) Monte-Carlo radiative transfer, one assumes that the number of photon packets N_i emitted by an atmospheric cell is proportional to its luminosity L_i ([Pinte et al. 2006](#); [Lee et al. 2017](#)):

$$N_i = \left(\frac{L_i}{L_{\text{tot}}} \right) N_{\text{tot}}, \quad (2.25)$$

with $L_{\text{tot}} = \Sigma L_i$ the total luminosity of the atmosphere and $N_{\text{tot}} = \Sigma N_i$ the total number of emitted photon packets at a given wavelength. All photon packets have an equal weight $w_i = 1$, which quantifies how much a photon packet contributes to the final planet flux.

A downside of Equation 2.25 is that cells with a low luminosity (e.g., on the nightside of a tidally locked planet) are likely to be *undersampled* in the radiative transfer, leading to high stochastic noise. To circumvent this problem, composite biasing ([Baes et al. 2016](#)) can be applied. In this case, the number of photon packets originating from the i -th cell is

$$N_i = N_{\text{tot}} \left((1 - \xi) \frac{L_i}{L_{\text{tot}}} + \xi \frac{1}{n_{\text{cells}}} \right). \quad (2.26)$$

Here, $\xi \in [0, 1]$ is a scaling parameter and n_{cells} is the total number of atmospheric cells. Equation 2.26 is a compromise between non-biased Monte-Carlo radiative transfer ($\xi = 0$) and uniform sampling ($\xi = 1$), where each cell emits the same number of packets. To ensure that the total luminosity of the atmosphere is conserved, the packet weights must be adjusted according to

$$w_i = \frac{1}{(1 - \xi) + \xi \langle L_i \rangle / L_i}, \quad (2.27)$$

with $\langle L_i \rangle$ the average luminosity of all cells at the relevant wavelength.

In *non-biased* Monte-Carlo radiative transfer, the following relationship holds between the weight of the photon packets and the luminosity of their cell:

$$L_i = w_i \left(\frac{N_i}{N_{tot}} \right) L_{tot} \quad (2.28)$$

In what follows, we will show that this relation also holds for the *biased* radiative transfer. Invoking Equation 2.27, we find

$$\begin{aligned} \frac{L_i}{w_i} &= L_i \left((1 - \xi) + \xi \frac{\langle L_i \rangle}{L_i} \right) \\ &= (1 - \xi) L_i + \xi \langle L_i \rangle \\ &= L_{tot} \left((1 - \xi) \frac{L_i}{L_{tot}} + \xi \frac{\langle L_i \rangle}{L_{tot}} \right) \\ &= \left(\frac{L_{tot}}{N_{tot}} \right) N_i, \end{aligned} \quad (2.29)$$

where the final equality was obtained from Equation 2.26. Moving the weight to the right-hand side yields the desired result. Hence, it holds for any value of ξ that

$$w_i = \left(\frac{N_i}{N_{tot}} \right) \left(\frac{L_{tot}}{L_i} \right). \quad (2.30)$$

Plugging Equation 2.24 into this expression, we find that the weight associated with a photon packet emitted from the i -th atmospheric cell is equal to

$$w_i = \left(\frac{N_i}{N_{tot}} \right) \left(\frac{L_{tot}}{4\pi\rho_i V_i \kappa_\lambda B_\lambda(T)} \right). \quad (2.31)$$

In the case of pure absorption, the “peel-off” weight $w_{po,i}$ of a photon packet as it escapes from the planet atmosphere along the line of sight is (Lee et al. 2017)

$$w_{po,i} = \frac{1}{4\pi} w_i e^{-\tau} = \left(\frac{N_i}{N_{tot}} \right) \left(\frac{L_{tot}}{16\pi^2 \rho_i V_i \kappa_\lambda B_\lambda(T)} \right) e^{-\tau}, \quad (2.32)$$

with $1/4\pi$ a factor accounting for isotropic emission and τ the optical depth encountered by the photon packet along the line of sight. To account for Doppler shifts due to winds and rotation, we again shift the opacities in each atmospheric cell according to Equation 2.6. Finally, the total emitted flux (with units $\text{erg}/\text{cm}^2/\text{s}/\text{cm}$) of the planet is obtained from

$$F_\lambda = \left(\frac{L_{tot}}{\pi R_p^2} \right) \left(\sum_j^{N_{tot}} w_{po,j} \right), \quad (2.33)$$

where R_p denotes the planet radius. Using Equation 2.33 it is also possible to compute a 3D contribution function for the planet. A contribution function (e.g., Lothringer et al.

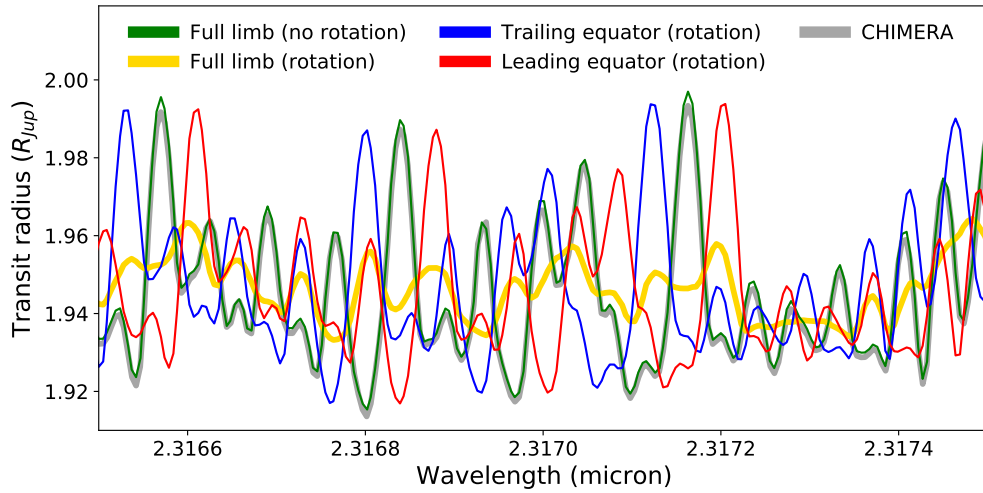


Figure 2.4: Transmission spectra of the 1D atmosphere used to benchmark gCMCRT with CHIMERA. The green curve shows the spectrum of the static atmosphere ($v_{\text{LOS}} = 0$ km/s), while the yellow curve denotes the spectrum obtained when Doppler shifts due to rotation are taken into account. In the latter case, the red and blue curves represent the contributions from the trailing and leading equator (see Figure 2.2), respectively. The spectrum computed with the 1D radiative transfer code CHIMERA is plotted in grey.

2018; Mollière et al. 2019) indicates from which atmospheric cells the observable flux is originating, and thus which regions are probed by the observation. To compute the emission contribution function, one can evaluate Equation 2.33 for each atmospheric cell *separately*, which gives an emergent flux $F_{\lambda}(\alpha, \varphi, z)$ for each latitude, longitude, and altitude.

2.2.5 Benchmarking tests

Transmission benchmark

In this section, we will demonstrate that the high-resolution mode of gCMCRT works correctly in the limit of a uniform, 1D atmosphere. Our task here is to show that the high-resolution opacity tables are properly evaluated and that the Doppler shifts resulting from Equation 2.5 are correctly implemented. To this end, we generate a simple model atmosphere with 16 latitudes, 32 longitudes and 100 vertical levels, containing H_2 , He, H_2O and CO. We adopt uniform number fractions $n_{\text{H}_2} = 0.86$, $n_{\text{He}} = 0.14$, $n_{\text{H}_2\text{O}} = 0.001$ and $n_{\text{CO}} = 0.01$, and we use a mean-molecular weight of $2.3 m_{\text{H}}$ (with m_{H} the mass of a hydrogen atom). The atmosphere extends from $P = 200$ bar (bottom) to $P = 10^{-8}$ bar (top) and has a uniform temperature of 2000 K. Furthermore, $R_0 = 1.76R_{\text{Jup}}$ and $(R_0 + z_{\text{max}}) = 2.05R_{\text{Jup}}$. Also, we assume that the planet has the same orbital period as WASP-76b (1.81 days), such that the rotational velocity at the equator is ± 5.3 km/s.

As shown in Figure 2.4, we compute a number of spectra with gCMCRT in a very narrow region near 2.3 micron. Additionally, we employ the 1D, plane-parallel radiative transfer code CHIMERA (Line et al. 2013, 2014) – which uses the same opacities – to compute the spectrum of the associated 1D atmosphere. In the radiative transfer, we account for the opacities of H_2O (Polyansky et al. 2018) and CO (Li et al. 2015), taken from the ExoMol database (Tennyson et al. 2020), as well the continuum due $\text{H}_2\text{-H}_2$ and $\text{H}_2\text{-He}$ collision-induced ab-

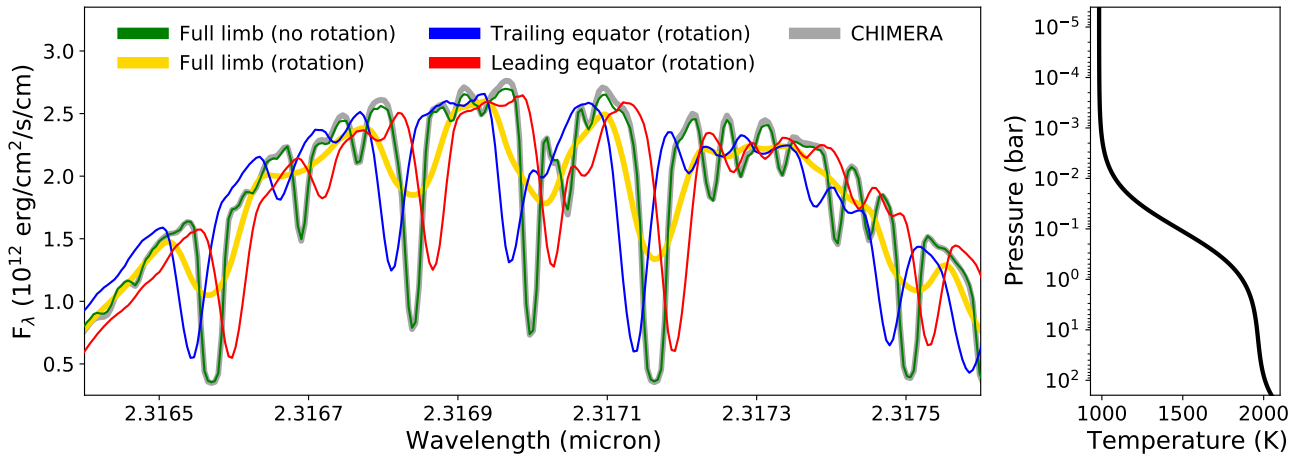


Figure 2.5: Left: Emission spectra of the 1D atmosphere used to benchmark gCMCRT with CHIMERA. The green curve shows the spectrum of the static atmosphere ($v_{\text{LOS}} = 0$ km/s), while the yellow curve denotes the spectrum obtained when Doppler shifts due to rotation are taken into account. In the latter case, the red and blue curves represent the contributions from the trailing and leading equator (see Figure 2.2), respectively. The spectrum computed with the 1D radiative transfer code CHIMERA is plotted in grey. **Right:** The pressure-temperature profile of the benchmark atmosphere.

sorption (Borysow et al. 2001; Borysow 2002; Gordon et al. 2017). Figure 2.4 demonstrates that there is a good agreement between the static Monte-Carlo spectrum, with $v_{\text{LOS}} = 0$ km/s in every cell, and the spectrum obtained from CHIMERA. Small differences are likely due to the way in which (the altitudes of) atmospheric levels are defined in the respective codes.

At high resolution, the transmission spectrum dramatically changes once gCMCRT accounts for the Doppler shifts due to planetary rotation. In this case, the spectrum can be interpreted as an average over the four limb sectors (Figure 2.2), each with their own effective velocity shift and line widths. The contributions from the trailing and leading equator are shown in Figure 2.4 as well. The trailing equator is blueshifted, because it rotates towards the observer. On the other hand, the leading equator is redshifted because it rotates away. The lines in both spectra are slightly less sharp compared to those of the static atmosphere, because there exists a slight dispersion in the line-of-sight velocities across the sectors.

Cross-correlating the equatorial spectra with the spectrum of the static atmosphere produces velocity shifts of ± 5.1 km/s, which is in agreement with the orbital period of the planet. Note that one would expect these values to be slightly smaller than ± 5.3 km/s, because the equatorial sectors defined in this work encompass all latitudes between ± 45 degrees.

Emission benchmark

We also perform a benchmark test in emission, similar to the work described in the previous paragraph. One change we make to the 1D model, however, is that we use a non-isothermal temperature profile. This is because an isothermal atmosphere (with no scattering) does not give rise to any spectral features – the spectrum will just resemble that of a black body. As

shown in Figure 2.5, our temperature profile drops from ~ 2000 K at high pressures to ~ 1000 K at lower pressures. The other atmospheric parameters are the same as for the transmission benchmark.

Figure 2.5 shows the gCMCRT and the CHIMERA spectra. Again, there is good agreement between both models. The emission spectra show *absorption* features because the models have a negative lapse rate. That is, at wavelengths where the opacity is *higher* (i.e., inside line cores), the emitted flux originates from *higher* altitudes in the atmosphere where the temperature is *lower*. On the other hand, if the lapse rate was positive (corresponding to a temperature inversion), the spectrum would show emission features.

In contrast to transmission, where the spectrum originates from a thin atmospheric limb, the emission spectrum emerges from the *entire* planet disk. This is why the spectra of the trailing and leading equator (which now cover 25% of the planet disk), appear more broadened compared to the transmission spectrum. The sectors span a larger area, so the variance in the Doppler shifts associated with a sector is also larger. Within a sector, the Doppler shifts due to rotation range from 0 km/s at the disk center to ± 5.3 km/s at the edge.

2.3 Reducing high-resolution observations

In this section, we will describe a typical data-reduction process for high-resolution observations. As an example, we consider observations taken by the IGRINS spectrograph on GEMINI-S (see also Appendix A). The instrument has a spectral resolution of $\sim 45,000$, while simultaneously covering the H and K bands between 1.42 and 2.42 microns (Levine et al. 2018; Line et al. 2021). We assume that the “raw data” have already been pre-processed by a pipeline of the observatory. In the case of IGRINS, this is the IGRINS pipeline package⁴ (PLP, Sim et al. 2014).

2.3.1 Producing a data cube

The PLP outputs separate files for each band and each integration. Each integration has a time stamp (in UTC) and a signal-to-noise (SNR) value associated with it. The goal now is to merge all data into a data cube $X(k, \lambda, \phi)$ that contains fluxes as a function of spectrograph order k , wavelength λ , and orbital phase ϕ . To this end, we carry out the following steps:

- Concatenating the H-band and the K-band data for each integration to obtain a single spectrum per time stamp.
- Determining the *orbital phases* of the planet associated with each data frame⁵. This can be done based on the location of the observatory (latitude, longitude, and altitude), the known time of the primary transit, and the time stamp of the integration. The time of the primary transit can be looked up on the NASA exoplanet archive⁶.
- Inferring the *barycentric velocities* associated with each data frame, based on the coordinates (RA, DEC) of the target and the time stamp of the integration⁷. The barycentric velocity manifests as an additional contribution to the Doppler shift of the planet

⁴PLP is publicly available from github.com/igrins/plp

⁵In Python, one can use the `coordinates.EarthLocation` and `Time` classes from the `astropy` library.

⁶exoplanetarchive.ipac.caltech.edu/cgi-bin/TransitView/nph-visibletbls?dataset=transits

⁷In Python, one can use the `SkyCoord` class from the `astropy` library.

spectrum, and has to be accounted for when transforming the observation into the rest frame of the exoplanet.

- Removing unwanted orders with low SNR values, given a certain threshold (typically ~ 100).
- Performing a wavelength calibration. To this end, we regard the frame taken closest in time to the sky frame as the “true” spectrum. Throughout the observation, the spectrum may undergo slight aberrations as a result of instrumental instabilities. In order to define all spectra on a common wavelength axis, we shift and rescale each frame by fitting it to the “true” spectrum.

2.3.2 Singular value decomposition of the data cube

The product of the wavelength calibration is a data cube $X(k, \lambda, \phi)$ in which all spectra are defined on the same wavelength axis. These fluxes are a combination of the stellar spectrum, telluric absorption (especially in the infrared), and the planet signal. In order to extract the planet signal from the data, we perform a singular value decomposition (SVD). SVD leverages the fact that stellar and telluric lines remain *stationary* during the observation, while the spectrum of the planet undergoes a Doppler shift induced by orbital motion. In data-reduction pipelines, SVD is typically treated as a black box. The goal of this section is to provide more insight into the theory behind this technique (e.g., [Blum et al. 2020](#)).

SVD is performed on each spectrograph order separately. Let $X_i = X(k_i, \lambda, \phi)$ be the matrix associated with the i -th order of the instrument. X_i is an $m \times n$ matrix, containing fluxes at m different time stamps (rows) and n different wavelengths (columns), with $m \ll n$. The SVD⁸ of X_i is now given by

$$X_i = U \Sigma V^T, \quad (2.34)$$

or, more verbosely,

$$\underbrace{\begin{bmatrix} - & x_1 & - \\ - & x_2 & - \\ & \vdots & \\ - & x_m & - \end{bmatrix}}_{\substack{m \text{ spectra with} \\ n \text{ wavelength points}}} = \underbrace{\begin{bmatrix} | & | & & | \\ u_1 & u_2 & \dots & u_m \\ | & | & & | \end{bmatrix}}_{\substack{m \times m \text{ matrix of} \\ \text{“eigen timeseries”}}} \underbrace{\begin{bmatrix} \sigma_1 & 0 & \dots & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ 0 & 0 & \dots & \sigma_m & \dots & 0 \end{bmatrix}}_{\substack{m \times n \text{ matrix with} \\ \text{singular values}}} \underbrace{\begin{bmatrix} | & | & & | \\ v_1 & v_2 & \dots & v_n \\ | & | & & | \end{bmatrix}^T}_{\substack{n \times n \text{ matrix with} \\ \text{“eigen fluxes”}}} \quad (2.35)$$

Here, U and V are unitary matrices, such that $U^T U = U U^T = I_m$ and $V^T V = V V^T = I_n$. This means that the rows and columns of U and V are orthogonal, and thus linearly independent. Furthermore, Σ is a (rectangular) diagonal matrix, containing m singular values in its first m columns. These are ordered such that $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_m \geq 0$. When defined in this way, the SVD of a matrix is *unique* and guaranteed to exist (e.g., [Blum et al. 2020](#)).

Equation 2.35 can also be written as

$$X_i = \sum_{j=1}^m \sigma_j \left(\vec{u}_j \otimes \vec{v}_j \right) \equiv \sum_{j=1}^m \sigma_j A_j, \quad (2.36)$$

⁸In Python, one can numerically compute the SVD of a 2D matrix with the function `numpy.linalg.svd`

with $\otimes$ denoting the outer product and A_j a rank-1 matrix. The rank of A_j is unity because all columns are linearly dependent. This is because every column of A_j is obtained by multiplying the vector $\vec{u}_j$ with a different component of $\vec{v}_j$. All in all, Equation 2.36 demonstrates that SVD allows to write a matrix as *a sum of rank-1 matrices, with the scalar coefficients being the singular values*. We will call the terms in this sum the “SVD components” of X_i .

To obtain a rank- ℓ approximation of X_i , one performs the sum

$$X_i \approx \sum_{j=1}^{\ell} \sigma_j A_j, \quad (2.37)$$

in which only the first ℓ principal components (multiplied by their singular value) are in-

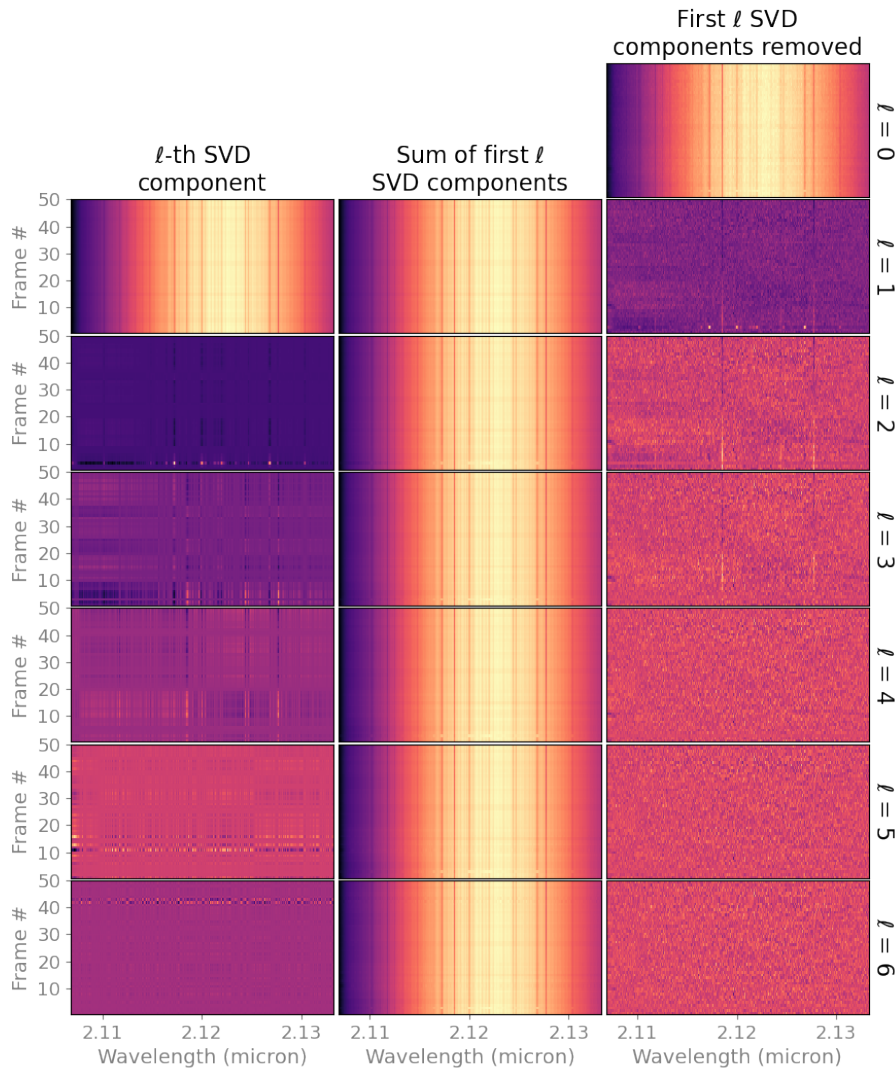


Figure 2.6: Visualisation of singular value decomposition (SVD). The panel in the top right contains wavelength-calibrated data from one of the K-band orders of Gemini-S/IGRINS (see Appendix A). The left column shows the largest six SVD components of this data matrix. The middle column shows the sum of these components (i.e., Equation 2.37 plotted for different values of ℓ), while the right column shows the residual matrix that results from subtracting the SVD components from the data (i.e., Equation 2.38 plotted for different values of ℓ). The residual matrix contains the planet signal, buried in photon noise. Cross-correlation with a template needs to be performed to recover the planet signal.

cluded. Because the singular values are ordered from large to small, the dominant features of X_i are contained in the first few principal components.

By construction, a single principal component is effective at capturing strong, stationary features in X_i (which do not change with either time or wavelength) as all columns of A_j scaled versions of each other. Therefore, the first few (and largest) principal components of A_j capture the planet and telluric lines, while the smaller components contain the weaker, time-varying planet signal. To isolate the planet signal from the data, we can discard the first ℓ principal components, and retain the smaller ones. That is,

$$X_i^{\text{planet}} = \sum_{j=\ell}^m \sigma_j A_j = X_i - \sum_{j=1}^{\ell} \sigma_j A_j = X_i - X_i^{\text{star+tellurics}}. \quad (2.38)$$

There is no a priori rule for how many principal components to remove from the data, but a typical choice is 4 or 5 (e.g., [Line et al. 2021](#); [Brogi et al. 2023](#)). A too low value of ℓ leaves too much stellar and telluric contamination, while a too high value potentially removes some of the planet signal, affecting the planet detection significance ([Holmberg & Madhusudhan 2022](#)). Some observational studies have also optimised the number of removed components per order (e.g., [Sánchez-López et al. 2022](#)).

2.3.3 Computing cross-correlation (CCF) maps

In high-resolution spectroscopy, the planet spectrum is generally buried in noise – see the bottom-right panel of Figure 2.6. Therefore, the information from *all* spectral features needs to be *combined* in order to recover the planet signal. A common way to do this is by cross-correlating the observational data with an atmospheric template ([Snellen et al. 2010](#); [Brogi et al. 2012](#)). The template can be a modelled spectrum of the planet, or a mask that is nonzero at the expected line positions and zero at other wavelengths (e.g., [Hoeijmakers et al. 2019](#); [Ehrenreich et al. 2020](#)). The resulting cross-correlation function (CCF) is a similarity measure: the better the overlap between the features (buried) in the data and those in the template, the higher the value of the CCF.

Given a set of exoplanet spectra $\vec{x}(\phi)$ at different orbital phases ϕ (either in transmission or emission) and a template $\vec{T}(v)$, the CCF is defined as the inner product of the two:

$$\text{CCF}(\phi, v) = \sum_{j=1}^{N_\lambda} x_j(\phi) T_j(v), \quad (2.39)$$

where the sum is performed over all N_λ wavelength points. Furthermore, v is the velocity (RV) by which the template is (Doppler-)shifted. An example of a CCF map can be found in the top panel in Figure 2.7. It shows the iron absorption signal of WASP-121b presented in [Gibson et al. \(2020\)](#).

CCF maps of limb sectors (for simulated data)

This paragraph pertains to computing CCF maps based on *transmission spectra* modelled with gCMCRT. Because gCMCRT allows to compute spectra for different limb sectors, we can also obtain separate CCF maps for these regions. In what follows, we will drop the dependencies of the CCF on ϕ and v for notational convenience.

Because cross-correlation is a linear operation, we can express the CCF map of the full atmospheric limb as the average of the CCF maps associated with the individual limb sectors $\mathcal{S}_i$. Since the transit depth is proportional to the effective area of the planet, we can substitute Equation 2.10 into Equation 2.39 to obtain

$$\text{CCF} = \sum_{j=1}^{N_\lambda} \left(\sum_{i=1}^{N_s} \beta_i x_{i,j} \right) T_j, \quad (2.40)$$

with $x_{i,j}$ the spectral value of sector $\mathcal{S}_i$ at wavelength j . Rearranging gives

$$\text{CCF} = \sum_{i=1}^{N_s} \beta_i \cdot \left(\sum_{j=1}^{N_\lambda} x_{i,j} T_j \right) = \sum_{i=1}^{N_s} \beta_i \cdot \text{CCF}_i, \quad (2.41)$$

with CCF_i the cross-correlation that is obtained when multiplying the spectrum of sector $\mathcal{S}_i$ with the template. By analogy with Equation 2.11, it holds that

$$\text{CCF} = \langle \text{CCF}_i \rangle, \quad (2.42)$$

when all sectors have the same area, as is the case in this work. Equation 2.42 is an important result, because it allows us to decompose the CCF map of the atmosphere into multiple contributions that are easier to interpret than the signal of the full limb. The total CCF is simply proportional to the sum of these contributions.

Choice of CCF

On a final note, we remind the reader that Equation 2.39 is not a unique definition of the CCF. Another frequently used expression is the Pearson correlation coefficient, where the inner product from Equation 2.39 is normalised by the square root of the product of the spectrum and template variances – see Appendix B in Hoeijmakers et al. (2019) for further details. The Pearson correlation coefficient appears in the CCF-to-likelihood mapping (Brogi et al. 2018; Gibson et al. 2020) that is used in high-resolution retrieval analyses (e.g., Line et al. 2021; Van Sluijs et al. 2022).

In this work, we do not use the Pearson correlation coefficient because it does not satisfy Equation 2.41. This is because different sectors may have spectra with different variances, such that the associated normalisation factor changes for every sector, and may not be equal to that of the total CCF. Also, we want to be able to relate the strength of the CCF signal to the strength of the spectral lines across the orbit, and this assessment would become harder if we normalised the CCF at each orbital phase.

2.3.4 Computing K_p - V_{sys} maps

Often, the CCF signals associated with individual phases are not strong enough to confidently detect the planet. Hence, we must go one step further and *combine* the information from *all* orbital phases – effectively “collapsing” the CCF map. One way to do this is by constructing a K_p - V_{sys} map (e.g., Brogi et al. 2012; Birkby et al. 2013; Hoeijmakers et al. 2019), in which each point is obtained by performing a sum along the phase axis in the CCF space (see Figure 2.7).

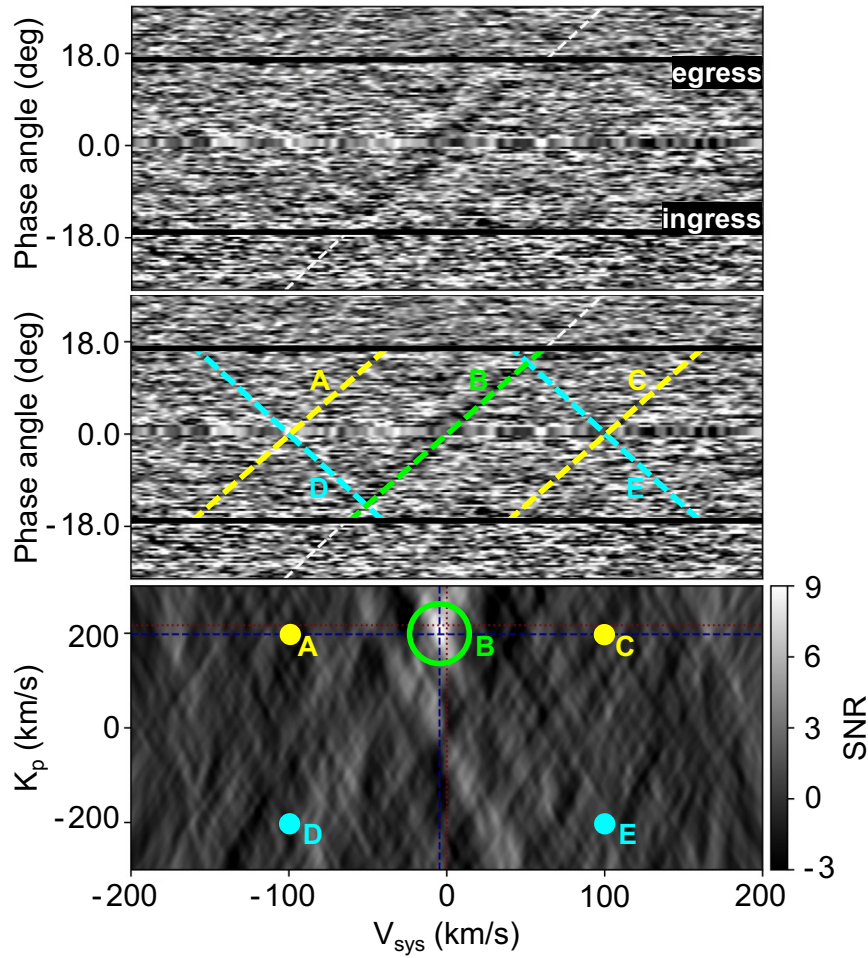


Figure 2.7: Plots showing the correspondence between a CCF map (top and middle panels) and a K_p - V_{sys} map (bottom panel). The top panel shows the Fe I absorption signal of the ultra-hot Jupiter WASP-121b (Gibson et al. 2020). The white dashes indicate the expected trail of the planet, based on its known (K_p, V_{sys}) values. The planet signal is visible between ingress and egress as a dark feature along this trail. A K_p - V_{sys} map is subsequently obtained by summing the signal along trails with different (K_p, V_{sys}) values, whereby each trail in the CCF map corresponds to one point in K_p - V_{sys} space – see Equation 2.43. Five of these trail-point pairs (labelled A–E) are visualised in the middle and bottom panels. When the CCF is summed along the “correct” trail (B), a peak will appear in the K_p - V_{sys} map. Figure adapted from Gibson et al. (2020).

To produce the CCF maps discussed in the previous section, we multiply the planet spectra $\vec{x}(\phi)$ at different orbital phases with a template $\vec{T}(v)$ shifted by many different velocities. For a planet with a circular orbit, there exists a simple relationship between its radial velocity v and its orbital phase angle $\phi \in [-180^\circ, 180^\circ]$:

$$v = V_{\text{sys}} + K_p \sin(\phi), \quad (2.43)$$

with V_{sys} the system velocity and K_p the velocity semi-amplitude. Through this equation, it is also possible to express the cross-correlation as a function of K_p and V_{sys} . That is, $\text{CCF} = \text{CCF}(K_p, V_{\text{sys}}, \phi)$. In practice, the cross-correlation is always a discrete function, so it can be represented by a cube of numbers $\text{CCF}_{j,k,l}$, where j , k and l denote the K_p , V_{sys} and ϕ axes, respectively.

In order to combine the spectra from all orbital phases, and obtain a single signal-to-noise ratio (SNR) for the *entire* observation, one typically co-adds the CCF values along the phase axis of the cube:

$$\text{SNR}(K_p, V_{\text{sys}}) \equiv \sum_{l=1}^{N_\phi} a (\text{CCF}_{j,k,l} - b), \quad (2.44)$$

with a a scaling factor and b a baseline (Hoeijmakers et al. 2015; Cabot et al. 2020). In the absence of atmospheric dynamics and planetary rotation, the SNR must acquire a maximum at the true (K_p, V_{sys}) values of the planet, when all CCF peaks in the data cube align. The value of this maximum is the SNR associated with the detection of the species whose absorption lines were included in the template. It should be stressed that the SNR is a *time-averaged* quantity, because we co-add the CCF values from different orbital phases.

In observations, the encountered SNR peak (e.g., dark blue dashes in the bottom panel of Figure 2.7) can be *offset* from the expected (K_p, V_{sys}) values of the planet (e.g., maroon dashes in Figure 2.7). A possible explanation for this is the 3D structure and dynamics of the atmosphere, as we will further discuss in Chapter 3.

K_p - V_{sys} maps of limb sectors (for simulated data)

As with the CCF map of the simulated gCMCRT transmission spectra, we can also express the SNR in terms of limb sectors. Plugging Equation 2.41 into Equation 2.44 yields

$$\begin{aligned} \text{SNR} &= \sum_{l=1}^{N_\phi} a \left[\left(\sum_{i=1}^{N_s} \beta_i \cdot \text{CCF}_{i,j,k,l} \right) - b \right] \\ &= \sum_{l=1}^{N_\phi} \left[a \sum_{i=1}^{N_s} \beta_i (\text{CCF}_{i,j,k,l} - b) \right] \\ &= \sum_{i=1}^{N_s} \left[\beta_i \sum_{l=1}^{N_\phi} a (\text{CCF}_{i,j,k,l} - b) \right] = \sum_{i=1}^{N_s} \beta_i \cdot \text{SNR}_i \end{aligned} \quad (2.45)$$

where we dropped the dependencies on K_p and V_{sys} . Furthermore, SNR_i is the signal-to-noise ratio associated with sector $\mathcal{S}_i$. Note that equation 2.45 only holds when the same values of a and b are used for every sector. Furthermore, when all limb sectors have the same area, we find that

$$\text{SNR} = \langle \text{SNR}_i \rangle, \quad (2.46)$$

where the angle brackets denote the average over the limb sectors.

Bibliography

- Adcroft A., Campin J.-M., Hill C., Marshall J., 2004, *Monthly Weather Review*, 132, 2845
 Baes M., Gordon K. D., Lunttila T., Bianchi S., Camps P., Juvela M., Kuiper R., 2016, *A&A*, 590, A55
 Birkby J. L., de Kok R. J., Brogi M., de Mooij E. J. W., Schwarz H., Albrecht S., Snellen I. A. G., 2013, *MNRAS: Letters*, 436, L35

- Blum A., Hopcroft J., Kannan R., 2020, Best-Fit Subspaces and Singular Value Decomposition (SVD). Cambridge University Press, p. 29–61, [doi:10.1017/9781108755528.003](https://doi.org/10.1017/9781108755528.003)
- Borysow A., 2002, *A&A*, 390, 779
- Borysow A., Jørgensen U. G., Fu Y., 2001, *J. Quant. Spectrosc. Radiative Transfer*, 68, 235
- Brogi M., Snellen I. A., De Kok R. J., Albrecht S., Birkby J., De Mooij E. J., 2012, *Nature*, 486, 502
- Brogi M., Jacobbe P., Guilluy G., de Kok R. J., Sozzetti A., Mancini L., Bonomo A. S., 2018, *A&A*, 615, A16
- Brogi M., et al., 2023, *AJ*, 165, 91
- Cabot S. H. C., Madhusudhan N., Welbanks L., Piette A., Gandhi S., 2020, *MNRAS*, 494, 363
- Constantin A., Johnson R. S., 2017, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 473, 20170063
- Ehrenreich D., et al., 2020, *Nature*, pp 1–7
- Fu Q., Liou K. N., 1992, Technical Report 22, On the Correlated k-Distribution Method for Radiative Transfer in Nonhomogeneous Atmospheres, <http://journals.ametsoc.org/jas/article-pdf/49/22/2139/3426108/1520-0469>. <http://journals.ametsoc.org/jas/article-pdf/49/22/2139/3426108/1520-0469>
- Gibson N. P., et al., 2020, *MNRAS*, 493, 2215
- Goody R., West R., Chen L., Crisp D., 1989, *J. Quant. Spectrosc. Radiative Transfer*, 42, 539
- Gordon I. E., et al., 2017, *J. Quant. Spectrosc. Radiative Transfer*, 203, 3
- Harada C. K., Kempton E. M. R., Rauscher E., Roman M., Malsky I., Brinjikji M., DiTomaso V., 2021, *ApJ*, 909, 85
- Hoeijmakers H. J., de Kok R. J., Snellen I. A. G., Brogi M., Birkby J. L., Schwarz H., 2015, *A&A*, 575, A20
- Hoeijmakers H. J., et al., 2019, *A&A*, 627, A165
- Holmberg M., Madhusudhan N., 2022, *AJ*, 164, 79
- Hood B., Wood K., Seager S., Collier Cameron A., 2008, *MNRAS*, 389, 257
- Kataria T., Showman A. P., Fortney J. J., Stevenson K. B., Line M. R., Kreidberg L., Bean J. L., Désert J.-M., 2015, *ApJ*, 801, 86
- Komacek T. D., Showman A. P., 2016, *ApJ*, 821, 16
- Lee E. K. H., Wood K., Dobbs-Dixon I., Rice A., Helling C., 2017, *A&A*, 601, A22
- Lee E. K. H., Taylor J., Grimm S. L., Baudino J.-L., Garland R., Irwin P. G. J., Wood K., 2019, *MNRAS*, 487, 2082
- Lee E. K. H., et al., 2022, *ApJ*, 929, 180
- Levine S., et al., 2018, in Takami H., Evans C. J., Simard L., eds, Vol. 10702, Ground-based and Airborne Instrumentation for Astronomy VII. SPIE, p. 26, [doi:10.1117/12.2312345](https://doi.org/10.1117/12.2312345), <https://www.spiedigitallibrary.org/conference-proceedings-of-spie/10702/2312345/IGRINS-at-the-Discovery-Channel-telescope-and-Gemini-South/10.1117/12.2312345.full>
- Li J., Goodman J., 2010, *ApJ*, 725, 1146
- Li G., Gordon I. E., Rothman L. S., Tan Y., Hu S.-M., Kassi S., Campargue A., Medvedev E. S., 2015, *ApJ Supplement Series*, 216, 15
- Line M. R., et al., 2013, *ApJ*, 775, 137
- Line M. R., Knutson H., Wolf A. S., Yung Y. L., 2014, *ApJ*, 783, 70
- Line M. R., et al., 2021, *Nature*, 598, 580
- Lions J.-L., Temam R., Wang S., 1992, *Nonlinearity*, 5, 237
- Lothringer J. D., Barman T., Koskinen T., 2018, *ApJ*, 866, 27
- Marley M. S., McKay C. P., 1999, *Icarus*, 138, 268
- Mihalas D., 1978, *Stellar Atmospheres*, 2 edn. Freeman, San Francisco
- Mollière P., Van Boekel R., Dullemond C., Henning T., Mordasini C., 2015, *ApJ*, 813, 47
- Mollière P., Wardenier J. P., van Boekel R., Henning T., Molaverdikhani K., Snellen I. A. G., 2019
- Noebauer U. M., Sim S. A., 2019, *Living Reviews in Computational Astrophysics*, 5, 1
- Parmentier V., Crossfield I. J. M., 2018, *Exoplanet Phase Curves: Observations and Theory*. Springer, p. 116, [doi:10.1007/978-3-319-55333-7_116](https://doi.org/10.1007/978-3-319-55333-7_116)
- Perna R., Menou K., Rauscher E., 2010a, *ApJ*, 719, 1421
- Perna R., Menou K., Rauscher E., 2010b, *ApJ*, 724, 313
- Pinte C., Ménard F., Duchêne G., Bastien P., 2006, *A&A*, 459, 797
- Polyansky O. L., Kyuberis A. A., Zobov N. F., Tennyson J., Yurchenko S. N., Lodi L., 2018, *MNRAS*, 480, 2597
- Rauscher E., Menou K., 2012, *ApJ*, 750, 96
- Sánchez-López A., Landman R., Mollière P., Casasayas-Barris N., Kesseli A. Y., Snellen I. A. G., 2022, *A&A*, 661, A78
- Showman A. P., Fortney J. J., Lian Y., Marley M. S., Freedman R. S., Knutson H. A., Charbonneau D., 2009, *ApJ*,

699, 564

Showman A. P., Lewis N. K., Fortney J. J., 2015, *ApJ*, 801, 95

Sim C. K., et al., 2014, *Advances in Space Research*, 53, 1647

Snellen I. A. G., De Kok R. J., De Mooij E. J. W., Albrecht S., 2010, *Nature*, 465, 1049

Steinacker J., Baes M., Gordon K. D., 2013, *Annual Review of A&A*, 51, 63

Stolker T., Min M., Stam D. M., Mollière P., Dominik C., Waters L. B. F. M., 2017, *A&A*, 607, A42

Tennyson J., et al., 2020, *J. Quant. Spectrosc. Radiative Transfer*, 255, 107228

Tinetti G., Tennyson J., Griffith C. A., Waldmann I., 2012, Water in exoplanets, [doi:10.1098/rsta.2011.0338](https://doi.org/10.1098/rsta.2011.0338)

Vallis G. K., 2017, Atmospheric and Oceanic Fluid Dynamics: Fundamentals and Large-Scale Circulation, 2 edn. Cambridge University Press, [doi:10.1017/9781107588417](https://doi.org/10.1017/9781107588417)

Van Sluijs L., et al., 2022, arXiv e-prints, [p. arXiv:2203.13234](https://arxiv.org/abs/2203.13234)

Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, *MNRAS*, 506, 1258

Whitney B. A., 2011, Bulletin of the Astronomical Society of India, 39, 101

Chapter 3

3D effects in ultra-hot Jupiters: An overview of observations and modelling studies

The material in this chapter is partly based on [Wardenier et al. \(2021\)](#) and [Wardenier et al. \(2023\)](#):

- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, MNRAS, 506, 1258
- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R. (submitted to MNRAS)

Abstract – In this chapter, we present a literature review of 3D effects in ultra-hot Jupiters (UHJs). Firstly, we describe four ways in which the “3D-ness” of UHJs manifests in high-resolution spectroscopy (HRS), and we discuss observational works that have reported these signatures. In the second half of the chapter, we summarise a number of 3D modelling studies that have simulated high-resolution spectra based on outputs of global circulation models (GCMs).

3.1 Observational signs of 3D structure

Over the past few years, both transmission and emission observations at high spectral resolution have led to insights about the 3D structure of UHJ atmospheres.

UHJs typically rotate by 25–30 degrees during transit (e.g., Chapter 5), thanks to their proximity to their host stars. At ingress, the leading limb (or *morning limb*) is largely comprised of dayside atmosphere, while the trailing limb (or *evening limb*) mainly covers the nightside. However, as the transit progresses, the dayside rotates into view on the trailing limb, and the nightside rotates into view on the leading limb (e.g., Chapter 5; [Ehrenreich et al. 2020](#); [Gandhi et al. 2022](#)). Because the terminator regions of UHJs are characterised by extreme thermochemical gradients, the planet spectrum can be expected to undergo observable changes over the course of the transit.

Whereas transmission spectra probe the *limb* of the atmosphere, emission spectra probe the entire planet *disk*. Just before/after transit ($\phi = 0^\circ$), most of the planet’s nightside is in view. At quadrature ($\phi = \pm 90^\circ$), half the dayside and half the nightside can be observed. Just before/after secondary eclipse ($\phi = 180^\circ$), the planet disk is almost fully comprised of dayside atmosphere. Furthermore, a common feature of UHJs is that they have thermal inversions on their daysides. On the nightside, the temperature is expected to decrease with altitude. Consequently, an emission spectrum will show *absorption* features when the nightside is in view, and *emission* features when the dayside is probed (e.g., [Pino et al. 2020](#); [Line et al. 2021](#)).

In what follows, we will discuss a number of HRS observations that have revealed signs of the “3D-ness” of UHJs. Broadly, these can be split into four categories (see Figure 3.1):

- (A) Spectral lines of a species showing *phase-dependent* Doppler shifts in the planetary rest frame (e.g., an increasing blueshift). This also leads to a peak offset from the expected planet position in the K_p - V_{sys} map.

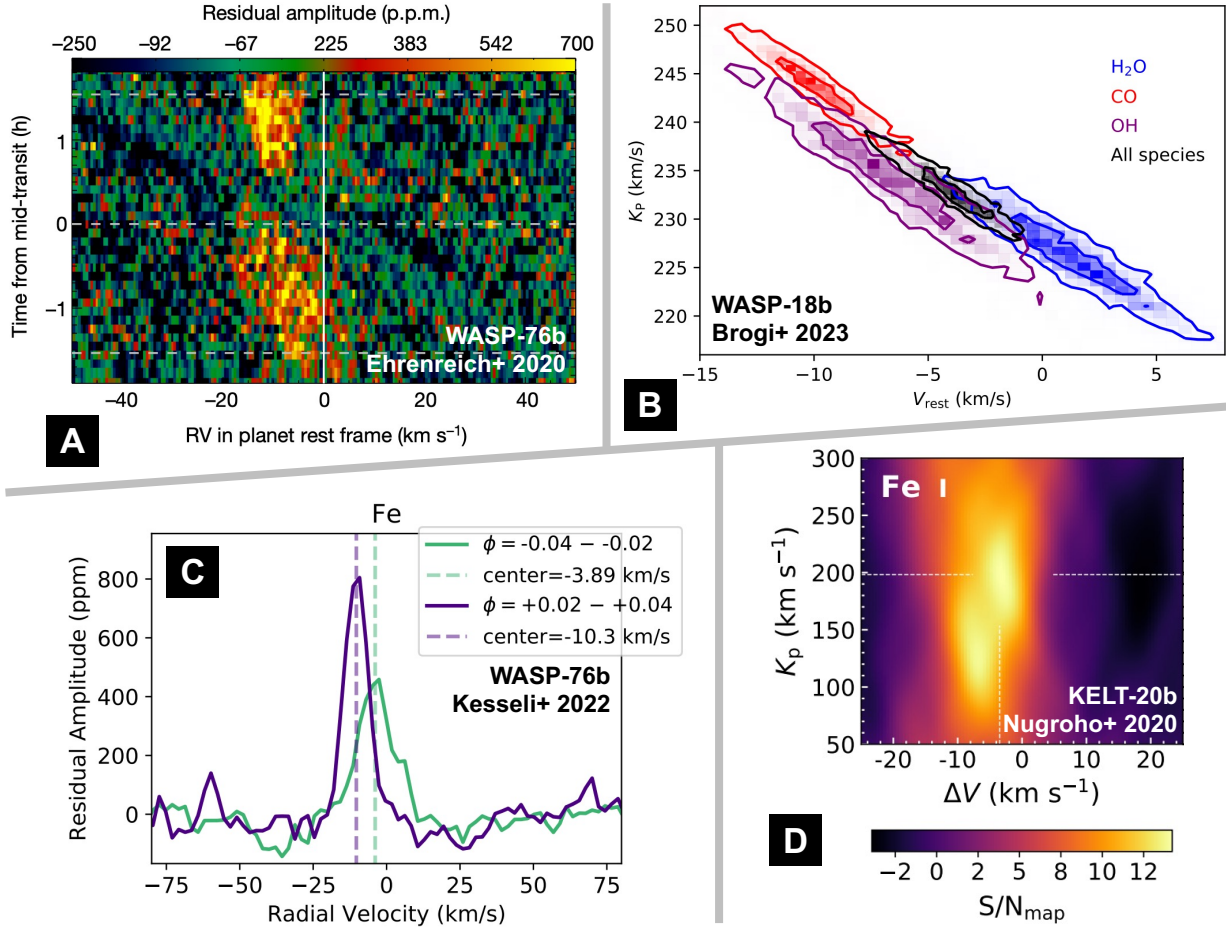


Figure 3.1: Observational examples of each of the four types of 3D effects discussed in this chapter. **(A)** CCF map showing the Doppler shift of the iron absorption lines of WASP-76b as a function of orbital phase during the transit (Ehrenreich et al. 2020). **(B)** K_p - V_{sys} map for H₂O, CO, and OH based on emission observations of WASP-18b. For each species, the detection peaks are located at different (K_p, V_{sys}) values (Brogi et al. 2023). **(C)** Average CCF signal for iron in the atmosphere of WASP-76b, during the first quarter (green curve) and final quarter (purple curve) of the transit (Kesseli et al. 2022). **(D)** K_p - V_{sys} map for iron based on transmission observations of KELT-20b. The map exhibits a “double-peak” structure (Nugroho et al. 2020).

- (B)** Different chemical species showing different Doppler shifts and different peak offsets in the K_p - V_{sys} map.
- (C)** Phase-dependent signal strengths. That is, the line contrast of the spectrum changes over the course of the transit/orbit.
- (D)** Detection peaks with complex shapes in the K_p - V_{sys} map, such as a “double-peak feature” or a diamond shape.

3.1.1 Phase-dependent Doppler shifts, and peak offsets in K_p - V_{sys} maps

From an observational standpoint, phase-resolving the signal of a planet with sufficiently high accuracy is a challenge. In most HRS datasets, all integrations need to be *combined* in order to achieve a significant detection (e.g., Figure 1.3). To the knowledge of the author,

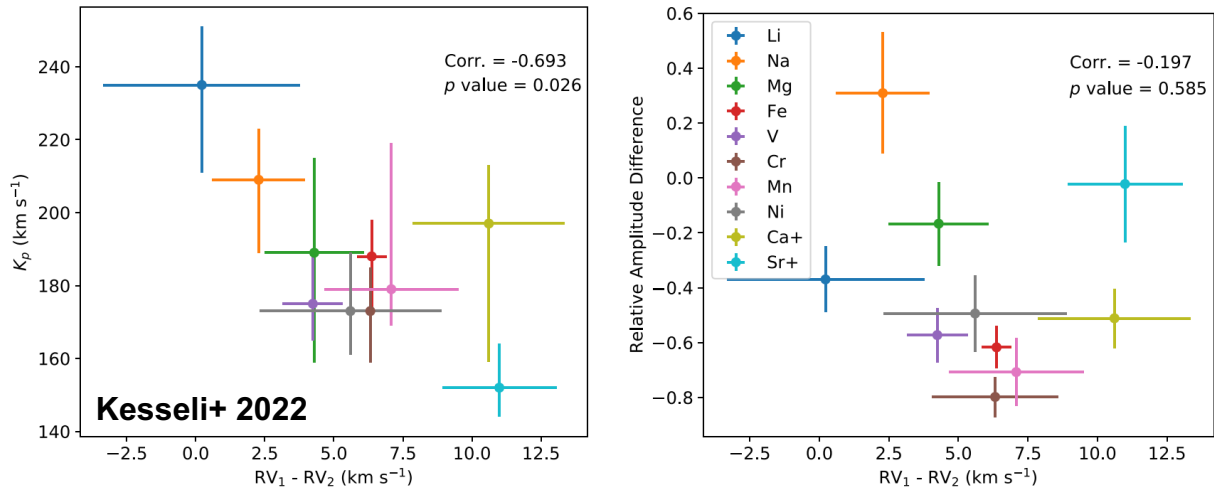


Figure 3.2: Plots showing the difference in net Doppler shift ($RV_1 - RV_2$) between the first and final quarter of the transit for ten refractory species in WASP-76b (Kesseli et al. 2022). $RV_1 - RV_2 > 0$ implies an increase in blueshift during the transit. The left panel shows the K_p coordinate of the detection peak in the $K_p - V_{\text{sys}}$ map plotted against $RV_1 - RV_2$. The right panel shows the relative difference in signal strength (i.e., the amplitude of the CCF) between the first and final quarter of the transit. A positive (*negative*) value means that the signal during the first quarter is stronger (*weaker*) than the signal during the final quarter.

only the neutral-iron (Fe I or Fe) signals of WASP-76b (Ehrenreich et al. 2020; panel A in Figure 3.1), WASP-121b (Borsa et al. 2021), and KELT-20b (Rainer et al. 2021) have been meaningfully constrained *at more than two orbital phases in transmission*.

The WASP-76b and WASP-121b datasets were obtained with VLT/ESPRESSO (Pepe et al. 2010), one of the most powerful telescope-spectrograph combinations in the world. For both planets, the CCFs show an increasing blueshift during the transit, with the peak position moving from about 0 km/s at ingress to about -10 km/s at egress in the planetary rest frame. Such signals are a clear hallmark of “3D-ness”, as they hint at the fact that a spatially varying limb region is probed (e.g., Chapter 4; Savel et al. 2022, Gandhi et al. 2022). The strong blueshift in the second half of the transit suggests that iron lines are predominantly probing the trailing limb, where planet rotation and the day-to-night flow both point towards the observer (hence causing a blueshift). We will further explore this effect in Chapters 4 and 6. The KELT-20b absorption signal published by Rainer et al. (2021) was based on five transits observed with HARPS-N. Rather than cross-correlating the data with a template model, they performed a line-fitting procedure to obtain the Doppler shift of the iron lines as a function of phase. When aggregated, the observations reveal a small blueshift (consistent with 0 km/s) during the transit. It increases to -10 km/s at egress, when only the trailing limb of the planet is blocking the star. Additionally, Rainer et al. (2021) found evidence for atmospheric variability across the different transits.

CCF trails that depart from 0 km/s in the planetary rest frame (as in panel A in Figure 3.1) will always result in a peak offset in the corresponding $K_p - V_{\text{sys}}$ map. This is because the $K_p - V_{\text{sys}}$ map inherently assumes that the *only* Doppler contributions are from the system velocity and the orbital motion of the planet. Therefore, if the Doppler shifts induced by planet rotation and atmospheric dynamics are nonzero, the map will factor these into the K_p and V_{sys} values, causing the detection peak to shift away from the true planet position. We refer to table 3.1 for a full overview of species and planets for which offsets in $K_p - V_{\text{sys}}$ maps, as well as other 3D effects, have been observed.

Table 3.1: Non-exhaustive overview of 3D-effects observed in the atmospheres of UHJs at high resolution. Planets are sorted by their equilibrium temperature $T_{\text{eq}} = T_{\text{star}} \sqrt{R/2a}$, with T_{star} the stellar effective temperature, R the stellar radius, and a the semi-major axis of the orbit, respectively. References to transmission and *emission* observations are printed in regular font and *italics*, respectively.

Planet (T_{eq})	Observed 3D effects with HRS
WASP-76b (2180 K)	Broadened Na I feature in transmission (Seidel et al. 2019); phase-dependent Doppler shift of Fe I lines during transit (Ehrenreich et al. 2020; Kesseli & Snellen 2021); different blueshifts measured for different species during transit (Tabernero et al. 2021; Kesseli et al. 2022); OH peak offset in K_p - V_{sys} map in transmission (Landman et al. 2021); H ₂ O and HCN peak offsets in K_p - V_{sys} map in transmission (Sánchez-López et al. 2022); different Doppler shift measured during first and final quarter of transit, for 11 different species (Kesseli et al. 2022); different H ₂ O and CO peak positions in K_p - V_{sys} map in emission (Yan et al. 2023); blueshifted absorption lines for different species in transmission (Azevedo Silva et al. 2022)
KELT-20b (2250 K)	Different Doppler shifts measured for different species (Casasayas-Barris et al. 2019); different blueshifts for Fe I and Fe II absorption lines (Stangret et al. 2020; Hoeijmakers et al. 2020a); change in signal strength of Fe II (Hoeijmakers et al. 2020a); Double-peak feature in K_p - V_{sys} map of Fe I (Nugroho et al. 2020; Rainer et al. 2021), Fe II and Cr I only detected after occultation, but not before (Borsa et al. 2022); Fe I signal stronger before occultation than after (Borsa et al. 2022);
WASP-121b (2360 K)	Fe I peak offset in K_p - V_{sys} map in transmission (Gibson et al. 2020); phase-dependent Doppler shift of Fe I lines during transit (Bourrier et al. 2020; Borsa et al. 2021); Peak offsets in K_p - V_{sys} map for different species in transmission (Merritt et al. 2021; Maguire et al. 2022); different blueshifts and offsets in K_p - V_{sys} map for different species – Sc II and Mg I are redshifted (Merritt et al. 2021); blueshifted absorption lines for several species (Ben-Yami et al. 2020; Hoeijmakers et al. 2020b; Azevedo Silva et al. 2022), broadened Na I feature in transmission (Hoeijmakers et al. 2020b; Seidel et al. 2023)
WASP-18b (2400 K)	Different H ₂ O, CO, and OH peak positions in K_p - V_{sys} map in emission (Brogi et al. 2023; Yan et al. 2023)
HAT-P-70b (2560 K)	Different blueshifts measured for different species (Bello-Arufe et al. 2022a)
WASP-189b (2640 K)	Different blueshifts measured for different species (Prinoth et al. 2022); redshifted Fe I and CO emission lines (Yan et al. 2022)
WASP-33b (2780 K)	TiO peak offset in emission, suggesting TiO-depleted hotspot (Cont et al. 2021); CO line contrast stronger after eclipse than before; eastward hotspot shift (Van Sluijs et al. 2022)
KELT-9b (4050 K)	Variation in depth of Fe I absorption features (Cauley et al. 2019); Blueshifted Fe II lines (Bello-Arufe et al. 2022b); anomalous Doppler shift of Fe I in emission (Pino et al. 2022)

Using the WASP-76b dataset from Ehrenreich et al. (2020), Kesseli et al. (2022) computed average CCFs over the first and final quarter of the transit for a large number of species, namely Fe, H, Li, Na, Mg, K, Ca II, V, Cr, Mn, Co, Ni, and Sr II¹. They found that *all* species except H and Li showed an *increase* in blueshift during the transit, leading to peak offsets in the corresponding K_p - V_{sys} maps. Figure 3.2 shows a summary of their work. It demonstrates that phase-dependent Doppler shifts are a universal feature for WASP-76b. Based on CARMENES data, Sánchez-López et al. (2022) applied a similar approach to the planet's H₂O and the HCN signals in the infrared. They also reported significant differences between the first and second half of the transit.

Finally, Pino et al. (2022) reported phase-dependent Doppler shifts in the Fe I signal of KELT-9b *in emission*, using CARMENES and HARPS-N observations. They found that the anomalous Doppler shift in the planetary rest frame could be reproduced by a model with a day-to-night flow of several km/s, in combination with the planet's day-night temperature contrast.

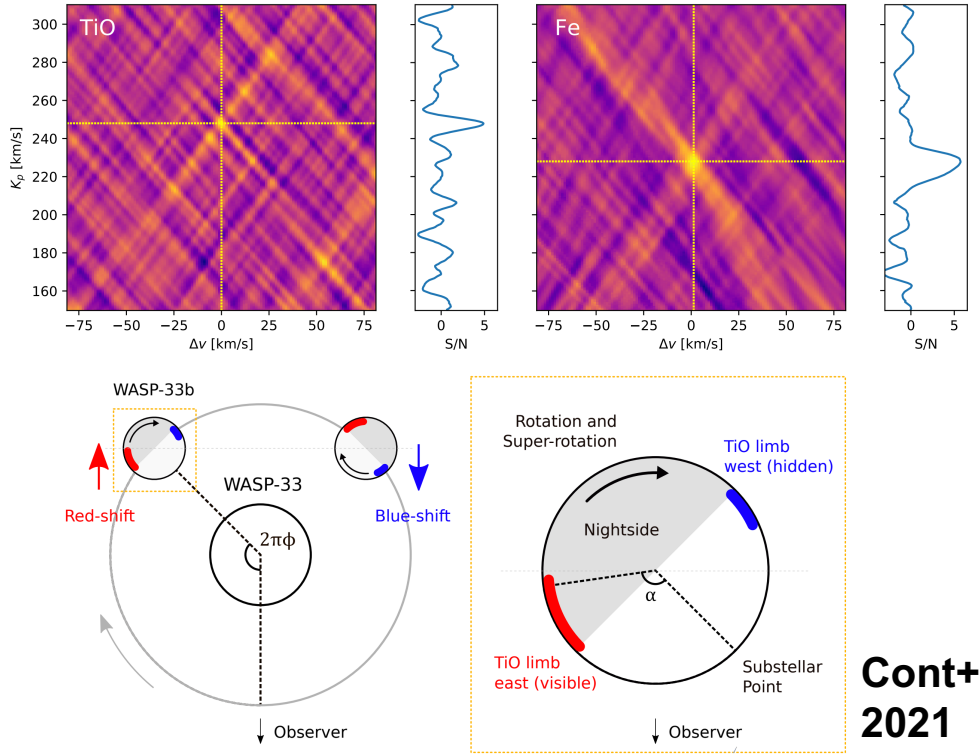
3.1.2 Different Doppler shifts and K_p - V_{sys} offsets for different species

Because each chemical species has its own opacity function and 3D spatial distribution across the planet, the spectral features of different atoms and molecules probe distinct regions of the atmosphere (see Chapter 6). As a result, they can be expected to show different Doppler shifts in the planetary rest frame.

As far as transmission observations are concerned, HRS has revealed species with different Doppler shifts in the atmospheres of WASP-76b (Tabernero et al. 2021, Kesseli et al. 2022, Azevedo Silva et al. 2022), KELT-20b (Casasayas-Barris et al. 2019; Stangret et al. 2020), WASP-121b (Merritt et al. 2021, Maguire et al. 2022), HAT-P-70b (Bello-Arufe et al. 2022b), and WASP-189b (Prinoth et al. 2022). In WASP-76b, for example, Tabernero et al. (2021) measured the Doppler shifts of the absorption lines of eleven species and found velocities ranging from -12.2 ± 1.4 km/s (Mn I line at 0.403 micron) to $+4.1 \pm 5.1$ km/s (Ca II K line at 0.393 micron). In WASP-121b, Merritt et al. (2021) found blueshifts for all species except Sc II and Mg I.

In emission, species with different Doppler shifts have been found in WASP-76b (Yan et al. 2023), WASP-18b (Brogi et al. 2023), and WASP-33b (Cont et al. 2021). Panel B in Figure 3.1 shows the 1σ and 2σ contours of the detection peaks associated with H₂O, CO, and OH in the K_p - V_{sys} map of WASP-18b. The different offsets are likely due to the fact that each species has its own 3D spatial distribution. The number fraction of CO should be uniform across the atmosphere, H₂O is prone to thermal dissociation on the dayside, while OH should occur in regions where H₂O is dissociated. For WASP-33b, Cont et al. (2021) found a strong (+17 km/s) offset of the TiO peak along the K_p axis. Conversely, the detection peak of iron was recovered at roughly the expected planet position in the K_p - V_{sys} map. Cont et al. (2021) showed that this discrepancy is consistent with thermal dissociation of TiO around the hotspot of the planet, such that its signal mainly emerges from the limb regions (see Fig. 3.3 for their observations and their corresponding toy model). At the limb, the Doppler contributions from planet rotation are such that they can emulate the signal of a planet with a *higher* orbital velocity and a *uniform* TiO abundance.

¹For notational convenience, we dropped the Roman numeral I for neutral atoms.



**Cont+
2021**

Figure 3.3: K_p - V_{sys} maps for TiO (top left) and iron (top right) based on pre- and post-eclipse emission spectra of WASP-33b (Cont et al. 2021). The detection peak of iron coincides with the expected (K_p , V_{sys}) values of the planet. The TiO peak, however, shows an offset of +17 km/s along the K_p axis. That is, based on the TiO lines in the emission spectrum, one would infer a higher orbital velocity for the planet. The bottom panels show the toy model presented by Cont et al. (2021) to explain this observation. If TiO is only present around the terminator (while being dissociated on the rest of the dayside), planet rotation will cause the TiO lines to pick up an extra redshift during pre-eclipse and an extra blueshift during post-eclipse, making it seem as if the planet is orbiting faster than it is in reality.

3.1.3 Phase-dependent signal strengths

Besides variations in Doppler shift, spectral features can also show variations in *strength* as a function of orbital phase. As we will see in Chapters 4 and 6, the strength of absorption lines in a transmission spectrum can be influenced by the planet's local temperature (via the scale height), the cloud-deck level, and projection effects related to the planet's rotation (Chapter 6). When it comes to emission spectra, the line strength mainly depends on the shape of the temperature profile that is being probed. An isothermal profile results in a lack of features (ignoring scattering), while profiles with steep vertical gradients give rise to strong absorption or emission lines. For UHJs, the line contrast can be expected to change drastically over the orbit, as different parts of the (thermally-inverted) dayside and the (non-inverted) nightside are in view at different orbital phases.

In transmission, changes in line strength have been observed for WASP-76b (Ehrenreich et al. 2020, Kesseli et al. 2022, Sánchez-López et al. 2022), KELT-20b (Hoeijmakers et al. 2020a), WASP-121b (Borsa et al. 2021), and KELT-9b (Cauley et al. 2019). Panel C in Fig. 3.1 shows the iron signal of WASP-76b (Ehrenreich et al. 2020; Kesseli et al. 2022) during the first and final quarter of the transit, respectively. It can be seen that the signal is almost twice as strong in the final quarter compared to the first quarter. Hoeijmakers et al. (2020a) found a

similar result for Fe II in KELT-20b. One explanation for this effect is a difference in temperature and scale height between the atmosphere’s trailing and leading limbs (see Chapter 4). If the trailing limb is hotter than the leading limb (e.g., due to a hotspot shift on the dayside), it will be more extended, resulting in a stronger line contrast over time. Alternatively, the leading limb could be depleted of iron due to condensation on the nightside of the planet (Ehrenreich et al. 2020).

In emission, variations in signal strength have so far been reported in KELT-20b (Borsa et al. 2022) and WASP-33b (Van Sluijs et al. 2022). Borsa et al. (2022) reported that the Fe I signal of KELT-20b is stronger *before* secondary eclipse than after, while the emission lines of Fe II and Cr I can only be detected *after* secondary eclipse and not before. These observations suggest that species have different spatial distributions across the dayside of the planet. For WASP-33b, Van Sluijs et al. (2022) found that the CO signal is stronger *after* the secondary eclipse than before. From comparisons to a GCM output, they found that the observations are consistent with an eastward hotspot shift on the planet. Inside the hotspot (eastern region of the dayside), thermal inversions are weaker compared to the planet’s western dayside. Therefore, the line contrast gets stronger when a larger portion of the western hemisphere is in view, which is after the secondary eclipse.

3.1.4 Double-peak features in K_p - V_{sys} maps

Anomalous Doppler shifts in the planetary rest frame do not only cause peak offsets in K_p - V_{sys} maps – they can also cause the detection peak to acquire a more complicated shape. If, due to rotation and atmospheric dynamics, the CCF trail of a planet can be equally well fit by multiple combinations of (K_p, V_{sys}) values, then this will lead to multiple maxima in the K_p - V_{sys} map (see panel D in Fig. 3.1 for an example). We will thoroughly study this effect in Chapters 4 and 6.

In transmission, double-peak features have been reported for Fe I on KELT-20b (Nugroho et al. 2020; Rainer et al. 2021). The fact that the feature was observed on multiple nights and with two different instruments boosts confidence that this is indeed an astrophysical signal. Nugroho et al. (2020) suggested that both peaks could be associated with the trailing and the leading limb, respectively. Both regions have different line-of-sight velocities due to the rotation of the planet. Rainer et al. (2021) observed five transits of KELT-20b and found that the peak feature changed between different nights, which could hint at atmospheric variability on the planet. Finally, the K_p - V_{sys} maps of WASP-76b (Kesseli et al. 2022) also show detection peaks with a more complicated structure, in particular for Mg, K, Ca II, V, Cr, and Mn.

3.2 3D modelling studies in high resolution

In this section, we will provide an overview of modelling studies that have explored the connection between the “3D-ness” of UHJs and their high-resolution spectra. In general, these studies employ a GCM to simulate the 3D temperature structure, chemistry, and dynamics of the planet. The GCM outputs are then post-processed by a radiative-transfer code to obtain transmission or emission spectra of the atmosphere (e.g., Chapter 2). The radiative transfer also accounts Doppler shifts due to rotation and dynamics.

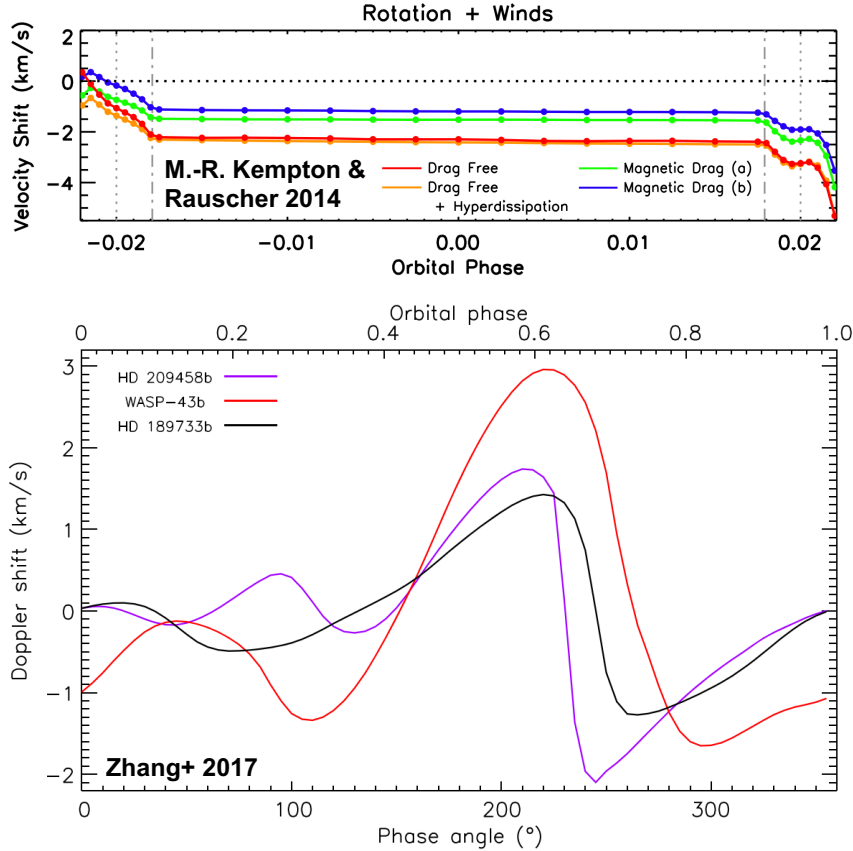


Figure 3.4: Examples of simulated CCF signals, obtained by post-processing the outputs of a 3D GCM. The top panel shows the phase-dependent Doppler shift of HD 209458b during transit (Miller-Ricci Kempton & Rauscher 2012), for modelling scenarios with magnetic drag (green and blue) and without magnetic drag (red and orange). The dash-dotted lines indicate the end of the ingress and the start of the egress, respectively. The bottom panel shows the Doppler shifts of simulated emission spectra of HD 189733b, HD 209458b, and WASP-43b along the entire orbit (Zhang et al. 2017).

3.2.1 Modelling transmission spectra of hot Jupiters

Following the first (-2 km/s) wind-speed measurement by Snellen et al. (2010) on HD 209458b, Miller-Ricci Kempton & Rauscher (2012) post-processed various 3D models of the planet to obtain its high-resolution transmission spectrum at different orbital phases between ingress and egress (see Fig. 3.4). The spectra were simulated at $R = 500,000$ between 2.291 to 2.350 micron (encompassing H_2O and CO lines), and subsequently binned down to the CRIRES resolution, $R = 100,000$. The study found that models with magnetic drag produced net blueshifts of about -1 km/s, and those without drag about -2 km/s, consistent with the result from Snellen et al. (2010). Furthermore, Miller-Ricci Kempton & Rauscher (2012) suggested that the Doppler shifts of individual absorption lines can be used to “resolve” the planet’s *vertical* wind profile, as lines with different strengths probe different layers of the atmosphere.

Showman et al. (2013) performed a similar study using the SPARC/MITgcm (Showman et al. 2009; see also Section 2.1). Contrary to Miller-Ricci Kempton & Rauscher (2012), they found that HD 209458b models *without* drag in the upper atmosphere gave blueshifts of -3 to -7 km/s. Rather, their simulations showed that models with drag timescales in the order of 10^4 – 10^6 s are needed to match the -2 km/s blueshift measured by Snellen et al.

(2010). Although the cause of the discrepancies between both works is not entirely clear, they are likely to originate from the different ways in which heating and cooling were treated in both GCMs. [Miller-Ricci Kempton & Rauscher \(2012\)](#) used a Newtonian relaxation scheme, while the SPARC/MITgcm employs non-grey radiative transfer.

A year later, [Rauscher & Kempton \(2014\)](#) explored the effect of (non-)synchronous rotation on the phase curves and high-resolution transmission spectra of hot Jupiters. They used models of HD 189733b and HD 209458b, with rotation rates equal to 0.5, 1, and 2 times the orbital period. They concluded that neither the phase curve, nor the Doppler signatures in the transmission spectrum could be used to constrain the planets' rotation rates. All models produced roughly the same net Doppler shifts, except for the fastest spinning HD 209458b model, which gave a stronger blueshift due to its hotter eastern limb.

[Kempton et al. \(2014\)](#) computed high-resolution transmission spectra for a grid of Jovian planets, with orbital periods ranging from 0.9 to 55 days. Additionally, they explored the impact of thermal inversions on transmission spectra. [Kempton et al. \(2014\)](#) found the strongest blueshifts (-3 km/s) for the most irradiated planets, while cooler planets on longer orbits gave no measurable Doppler shift. Moreover, the study concluded that the precise vertical shape of the temperature profile (i.e., inverted vs non-inverted) has no significant effect on a planet's transmission spectrum. Of course, the absolute temperature does matter, as it impacts the scale height.

More recently, [Wardenier et al. \(2021\)](#) and [Savel et al. \(2022\)](#) used GCM outputs to model the iron absorption signal of WASP-76b, also investigating the role of limb-asymmetries. We will discuss their work in Chapter 4.

3.2.2 Modelling emission spectra of hot Jupiters

[Zhang et al. \(2017\)](#) were the first to simulate high-resolution *emission* spectra based on 3D models of hot Jupiters. Their work featured three planets: HD 189733b, HD 209458b, and WASP-43b. For each planet, they computed the emission spectrum at different phases along the orbit, finding net Doppler shifts with magnitudes of 1–3 km/s in the planetary rest frame. For each model, [Zhang et al. \(2017\)](#) reported that the net Doppler shift obeys a “quasi-sinusoidal” behaviour as a function of orbital phase (see Fig. 3.4), due to the hotspot rotating towards (blueshift) and away (redshift) from the observer at different orbital phases. Also, they demonstrated that this net Doppler shift can be analytically approximated by adding up the different line-of-sight velocities across the planet disk, weighted by the local brightness of the atmosphere. That is, hotter regions contribute more strongly to the net Doppler shift, owing to the higher flux that they emit.

[Harada et al. \(2021\)](#) built on the work of [Zhang et al. \(2017\)](#), and specifically focused on the role of clouds in shaping the high-resolution emission spectra of hot Jupiters. To this end, they used a model with the same parameters as Kepler-7b. The work considered three scenarios: an atmosphere with (i) no clouds, (ii) post-processed clouds, and (iii) radiatively active clouds. In scenario (ii), the clouds were added to the model during post-processing. In scenario (iii), however, the clouds were added *inside* the GCM, such that the radiative feedback between the clouds and the temperature structure was accounted for. [Harada et al. \(2021\)](#) demonstrated that clouds mainly alter the spectrum of the planet through the temperature structure. While scenarios (i) and (ii) result in very similar spectra and net Doppler shifts, the active clouds in scenario (iii) introduce thermal inversions on the (initially non-inverted) dayside. Consequently, the emission spectrum contains a combination

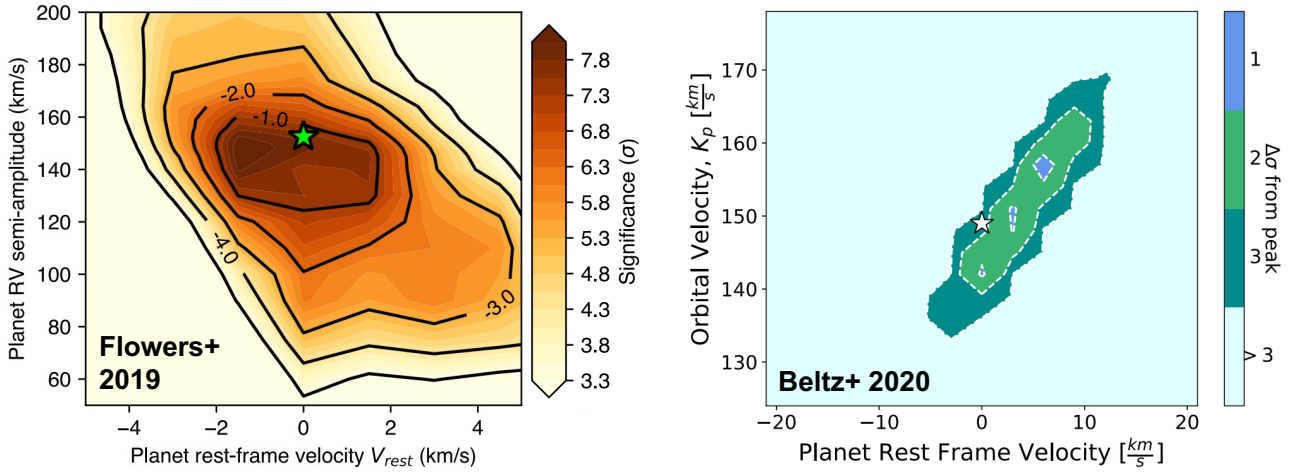


Figure 3.5: K_p - V_{sys} maps obtained after cross-correlating observational high-resolution data with a template based on a 3D GCM output. The left panel shows the detection peak for HD 189733b *in transmission* (Flowers et al. 2019), which has a maximum value of 8.2σ . The peak is consistent with the expected position of the planet (indicated by the green star) and a rest-frame velocity of 0 km/s within 1σ . The right panel shows the detection peak for HD 209458b *in emission* (Beltz et al. 2021). Its maximum value is 6.9σ . Because the observations cover a relatively small part of the orbit, there is a degeneracy between K_p and V_{sys} , resulting in an elongated peak shape.

of absorption and emission features, each with their own Doppler shift. This leads to more complicated behaviour in the CCF, as the net Doppler shift is very sensitive to the specific dayside regions that are in view. Additionally, Harada et al. (2021) showed that Doppler shifts become stronger when the active clouds have a greater vertical extent.

Malsky et al. (2021) explored the role of orbital inclination in shaping the emission spectra of hot Jupiters. To this end, they used a model with the atmospheric structure of Upsilon Andromedae b, considering both cloud-free and cloudy scenarios. Their work showed that with decreasing orbital inclination (where 90° means an edge-on configuration) four observable quantities also decrease: (i) the average continuum flux, (ii) the amplitude of the phase curve, (iii) the net Doppler shift of the spectrum, and (iv) the Doppler broadening of the spectral lines. Like Harada et al. (2021), they showed that the behaviour of the CCF becomes more intricate when clouds are considered, due to changes in the planet’s thermal structure.

3.2.3 Cross-correlating data with 3D models

Flowers et al. (2019) were the first to perform a direct comparison between spectra from a GCM and observational high-resolution data. In principle, cross-correlation templates that account for the 3D structure and dynamics of a planet should give rise to higher detection significances compared to 1D models, as they are a more realistic representation of *true* planet spectrum. Flowers et al. (2019) revisited infrared transit observations of HD 189733b from CRIRES, previously published by Brogi et al. (2016). They simulated atmospheres with 12 different rotation rates (keeping the orbital period fixed) and used the transmission spectra as cross-correlation templates to recover the planet signal in the real data. Using these 3D templates, Flowers et al. (2019) were able to constrain the rotation rate of the planet to 1.2–4.69 days, consistent with synchronous rotation (2.22 days). Moreover, for the best-fitting template, they recovered the planet signal at a *rest-frame velocity* of 0 km/s (see left

panel in Fig. 3.5). That is, no extra Doppler shift was required to match the model to the data, indicating that the GCM globally captured the dynamics of the planet. Remarkably, the detection significance of $\text{H}_2\text{O}+\text{CO}$ was found to be at most 8.2σ for the 3D templates, compared to 8.6σ for the best-fitting 1D template from Brogi et al. (2016). Switching off the winds in the 3D models resulted in an 8.7σ detection, albeit with the peak displaced in the K_p - V_{sys} map, as the templates no longer included effects of dynamics.

Beltz et al. (2021) performed a similar study in *emission* (see right panel in Fig. 3.5), using CRIRES data of HD 209458b originally presented in Schwarz et al. (2015). Besides computing 3D templates based on GCM outputs, they also generated hundreds of template models based on different 1D temperature profiles. Beltz et al. (2021) reported a 1.8σ improvement in the detection of $\text{H}_2\text{O}+\text{CO}$ when using a 3D template (6.9σ) instead of the best-fitting 1D template (5.1σ) – a much bigger improvement compared to Flowers et al. (2019). In principle, this is not surprising: Beltz et al. (2021) demonstrated that the strongest detection enhancement is achieved once the template is able to account for the planet’s 3D temperature profile, with smaller contributions from 3D chemistry and dynamics. Because an emission spectrum is a disk-average, the 3D temperature structure of a planet can give rise to complicated line shapes (e.g., a combination of absorption and emission features) that can inherently not be captured by a 1D model. In transmission, however, this is less of an issue as the spectral features are hardly sensitive to the precise shape of the temperature profile across the limb (Kempton et al. 2014).

3.2.4 The impact of magnetic effects on high-resolution spectra

Beltz et al. (2022) investigated the impact of magnetic drag on high-resolution *emission* spectra of UHJs. To this end, they computed phase-dependent spectra based on GCM outputs of WASP-76b with different magnetic-drag prescriptions: (i) no drag, (ii) a uniform drag timescale of 10^4 s, and (iii) active drag. While scenario (ii) cannot account for variations in magnetic drag across the planet, scenario (iii) relies on a local timescale that is calculated from the global magnetic field of the planet (assumed to be 3 G), the local mass density, the local temperature, and the local ionisation fraction. Overall, Beltz et al. (2022) found that the net Doppler shift of the planet follows a similar trend in each scenario, except for the nightside emission spectra being more redshifted in the models with magnetic drag. Furthermore, they demonstrated how cross-correlating spectra with templates that are *not* phase-dependent (i.e., which ignore the fact that different parts of the 3D temperature structure are in view at different orbital phases) can lead to wrong inferences of the atmosphere’s net Doppler shift.

Beltz et al. (2023) performed a similar study in *transmission*, making use of the same set of WASP-76b models. They computed transit spectra in three narrow wavelength ranges dominated by Fe, H_2O and CO lines, respectively. For each combination of species and model, except for the water signal in the active-drag model, Beltz et al. (2023) found that the spectra showed an increasing blueshift during the transit. In addition, they reported that the iron signal in the active drag model shows the same trend as the observation by Ehrenreich et al. (2020) (see panel A in Figure 3.1), suggesting that magnetic fields could also play a role in shaping the 3D structure of WASP-76b.

3.3 Summary

In Section 3.1, we discussed observational signs of the 3D structure of ultra-hot Jupiters (UHJs). In high-resolution spectroscopy (HRS), these manifest in four different ways: (i) phase-dependent Doppler shifts and peak offsets in K_p - V_{sys} maps, (ii) different Doppler shifts for different chemical species, (iii) phase-dependent signal strengths, and (iv) multi-peak features in K_p - V_{sys} maps. Table 3.1 provides a full overview of 3D effects that have so far been reported in the literature.

In Section 3.2, we showcased some of the capabilities of 3D modelling studies involving global circulation models (GCM). These studies are crucial for interpreting high-resolution observations, as 1D models are inherently unable to capture the full 3D temperature structure, chemistry, and wind-profile of a planet. In fact, observations and modelling studies often go hand in hand. The first wind speed measurement on HD 209458b by Snellen et al. (2010) led Miller-Ricci Kempton & Rauscher (2012) and Showman et al. (2013) run a GCM of the planet and constrain its atmospheric properties. In a similar spirit, the WASP-76b observations by Ehrenreich et al. (2020) motivated the work presented in Chapter 4.

Spectra generated from 3D models can also be used as cross-correlation templates. This is especially relevant in emission. If a planet disk features regions with and without thermal inversions, the emission spectrum will contain a mixture of absorption and emission features, which cannot be reproduced with a 1D model. Therefore, cross-correlating the data with a 3D template can significantly boost chemical detections.

Bibliography

- Azevedo Silva T., et al., 2022, *A&A*, 666, L10
 Bello-Arufe A., Cabot S. H. C., Mendonça J. M., Buchhave L. A., Rathcke A. D., 2022a, *AJ*, 163, 96
 Bello-Arufe A., Buchhave L. A., Mendonça J. M., Tronsgaard R., Heng K., Jens Hoeijmakers H., Mayo A. W., 2022b, *A&A*, 662, A51
 Beltz H., Rauscher E., Brogi M., Kempton E. M. R., 2021, *AJ*, 161, 1
 Beltz H., Rauscher E., Kempton E. M. R., Malsky I., Ochs G., Arora M., Savel A., 2022, *AJ*, 164, 140
 Beltz H., Rauscher E., Kempton E., Malsky I., Savel A., 2023, *arXiv e-prints*, p. arXiv:2302.13969
 Ben-Yami M., Madhusudhan N., Cabot S. H. C., Constantinou S., Piette A., Gandhi S., Welbanks L., 2020, Technical report, Neutral Cr and V in the atmosphere of ultra hot jupiter WASP-121 b, www.hsc-chemistry.com (arXiv:2006.05995v1), www.hsc-chemistry.com
 Borsa F., et al., 2021, *A&A*, 645, A24
 Borsa F., et al., 2022, *A&A*, 663, A141
 Bourrier V., et al., 2020, *A&A*, 635, A205
 Brogi M., de Kok R. J., Albrecht S., Snellen I. A. G., Birkby J. L., Schwarz H., 2016, *ApJ*, 817, 106
 Brogi M., et al., 2023, *AJ*, 165, 91
 Casasayas-Barris N., et al., 2019, *A&A*, 628, A9
 Cauley P. W., Shkolnik E. L., Ilyin I., Strassmeier K. G., Redfield S., Jensen A., 2019, *AJ*, 157, 69
 Cont D., et al., 2021, *A&A*, 651, A33
 Ehrenreich D., et al., 2020, *Nature*, pp 1–7
 Flowers E., Brogi M., Rauscher E., Kempton E. M.-R., Chiavassa A., 2019, *AJ*, 157, 209
 Gandhi S., Kesseli A., Snellen I., Brogi M., Wardenier J. P., Parmentier V., Welbanks L., Savel A. B., 2022, *MNRAS*, 515, 749
 Gibson N. P., et al., 2020, *MNRAS*, 493, 2215
 Harada C. K., Kempton E. M. R., Rauscher E., Roman M., Malsky I., Brinjikji M., DiTomasso V., 2021, *ApJ*, 909, 85
 Hoeijmakers H. J., et al., 2020a, *A&A*, 641, A120
 Hoeijmakers H. J., et al., 2020b, *A&A*, 641, A123

- Kempton E. M.-R., Perna R., Heng K., 2014, *ApJ*, 795, 24
- Kesseli A. Y., Snellen I. A. G., 2021, *ApJ*, 908, L17
- Kesseli A. Y., Snellen I. A. G., Casasayas-Barris N., Mollière P., Sánchez-López A., 2022, *AJ*, 163, 107
- Landman R., Sánchez-López A., Mollière P., Kesseli A. Y., Louca A. J., Snellen I. A. G., 2021, *A&A*, 656, A119
- Line M. R., et al., 2021, *Nature*, 598, 580
- Maguire C., Gibson N. P., Nugroho S. K., Ramkumar S., Fortune M., Merritt S. R., de Mooij E., 2022, *MNRAS*, 506, 3853
- Malsky I., Rauscher E., Kempton E. M. R., Roman M., Long D., Harada C. K., 2021, *ApJ*, 923, 62
- Merritt S. R., et al., 2021, *MNRAS*, 506, 3853
- Miller-Ricci Kempton E., Rauscher E., 2012, *ApJ*, 751, 117
- Nugroho S. K., Gibson N. P., de Mooij E. J. W., Watson C. A., Kawahara H., Merritt S., 2020, *MNRAS*, 496, 504
- Pepe F. A., et al., 2010, in *Ground-based and Airborne Instrumentation for Astronomy III*. SPIE, p. 77350F, doi:10.1117/12.857122, <https://ui.adsabs.harvard.edu/abs/2010SPIE.7735E..0FP/abstract>
- Pino L., et al., 2020, *ApJ*, 894, L27
- Pino L., et al., 2022, *A&A*, 668, A176
- Prinoth B., et al., 2022, *Nature Astronomy*, 6, 449
- Rainer M., et al., 2021, *A&A*, 649, A29
- Rauscher E., Kempton E. M. R., 2014, *ApJ*, 790, 79
- Sánchez-López A., Landman R., Mollière P., Casasayas-Barris N., Kesseli A. Y., Snellen I. A. G., 2022, *A&A*, 661, A78
- Savel A. B., et al., 2022, *ApJ*, 926, 85
- Schwarz H., Brogi M., de Kok R., Birkby J., Snellen I., 2015, *A&A*, 576, A111
- Seidel J. V., et al., 2019, *A&A*, 623, A166
- Seidel J. V., et al., 2023, *arXiv e-prints*, p. arXiv:2303.09376
- Showman A. P., Fortney J. J., Lian Y., Marley M. S., Freedman R. S., Knutson H. A., Charbonneau D., 2009, *ApJ*, 699, 564
- Showman A. P., Fortney J. J., Lewis N. K., Shabram M., 2013, *ApJ*, 762
- Snellen I. A. G., De Kok R. J., De Mooij E. J. W., Albrecht S., 2010, *Nature*, 465, 1049
- Stangret M., Casasayas-Barris N., Pallé E., Yan F., Sánchez-López A., López-Puertas M., 2020, *A&A*, 638, A26
- Tabernero H. M., et al., 2021, *A&A*, 646, A158
- Van Sluijs L., et al., 2022, *arXiv e-prints*, p. arXiv:2203.13234
- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, *MNRAS*, 506, 1258
- Yan F., et al., 2022, *A&A*, 661, L6
- Yan F., et al., 2023, *arXiv e-prints*, p. arXiv:2302.08736
- Zhang J., Kempton E. M.-R., Rauscher E., 2017, *ApJ*, 851, 84

Chapter 4

Decomposing the iron cross-correlation signal of the ultra-hot Jupiter WASP-76b in transmission using 3D Monte-Carlo radiative transfer

The material in this chapter is based on [Wardenier et al. \(2021\)](#):

– Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, MNRAS, 506, 1258

Abstract — Ultra-hot Jupiters are tidally locked gas giants with dayside temperatures high enough to dissociate hydrogen and other molecules. Their atmospheres are vastly non-uniform in terms of chemistry, temperature and dynamics, and this makes their high-resolution transmission spectra and cross-correlation signal difficult to interpret. In this chapter, we use the SPARC/MITgcm global circulation model to simulate the atmosphere of the ultra-hot Jupiter WASP-76b under different conditions, such as atmospheric drag and the absence of TiO and VO. We then employ a 3D Monte-Carlo radiative transfer code, HIRES-MCRT, to self-consistently model high-resolution transmission spectra with iron (Fe I) lines at different phases during the transit. To untangle the structure of the resulting cross-correlation map, we decompose the limb of the planet into four sectors, and we analyse each of their contributions separately. Our experiments demonstrate that the cross-correlation signal of an ultra-hot Jupiter is primarily driven by its temperature structure, rotation and dynamics, while being less sensitive to the precise distribution of iron across the atmosphere. We also show that the previously published iron signal of WASP-76b can be reproduced by a model featuring iron condensation on the leading limb. Alternatively, the signal may be explained by a substantial temperature asymmetry between the trailing and leading limb, where iron condensation is not strictly required to match the data. Finally, we compute the K_p – V_{sys} maps for the simulated WASP-76b atmospheres, and we show that rotation and dynamics can lead to multiple peaks that are displaced from zero in the planetary rest frame.

4.1 Introduction

One of the main goals associated with the characterisation of exoplanets is to quantify the abundances of chemical species in their atmospheres. Nonetheless, the inherent 3D structure of exoplanets complicates this endeavour. A suite of studies in low spectral resolution have demonstrated how interpreting observations with 1D models leads to *biased* inferences, both in the case of transmission spectra ([Line & Parmentier 2016](#); [MacDonald & Madhusudhan 2017](#); [Caldas et al. 2019](#); [Lacy & Burrows 2020](#); [MacDonald et al. 2020](#); [Pluriel et al. 2020](#)) and emission spectra ([Feng et al. 2016](#); [Blecic et al. 2017](#); [Taylor et al. 2020](#)). In high resolution, where individual spectral lines are resolved, the problem becomes even more intricate. This is because line shapes, depths and positions depend profoundly on the 3D thermal structure and chemical composition of the planet, as well as its wind profile and rotation ([Miller-Ricci Kempton & Rauscher 2012](#); [Showman et al. 2013](#); [Kempton et al. 2014](#); [Rauscher & Kemp-](#)

ton 2014; Zhang et al. 2017; Flowers et al. 2019; Harada et al. 2021; Seidel et al. 2020; Beltz et al. 2021; Keles 2021). Hence, comparing observational data to the wrong models may lead to wrong conclusions about the nature of the atmosphere. In fact, to extract the correct physical information, it is crucial to understand how spatial inhomogeneities across the atmosphere show up in transmission and emission spectra, and how these can be accounted for in models.

The aim of this chapter is to better understand how the 3D structure and dynamics of ultra-hot Jupiters impact their high-resolution transmission spectra, as well as the resulting cross-correlation signal. To this end, we feed the outputs of a 3D, non-grey global circulation model (GCM) into a Monte-Carlo radiative transfer code that is able to compute Doppler-shifted spectra at different stages during the transit. We apply our framework to the transiting ultra-hot Jupiter WASP-76b, for which Ehrenreich et al. (2020) and Kesseli & Snellen (2021) independently reported an asymmetric iron absorption signal (see Fig. 4.1) – an observation that could testify to 3D effects in the planet’s atmosphere. In Section 4.2, we briefly revisit the observation and discuss its current interpretation.

In Section 4.3, we outline how we generate our atmospheric structures with the GCM and how we use the Monte-Carlo code to compute transmission spectra. Additionally, we elaborate on the methods used to compute cross-correlation maps. The atmospheric structures and a number of spectra are presented in Section 4.4. Subsequently, in Sections 4.5 and 4.6, we present the cross-correlation maps and we attempt to link their behaviour to the physics of the atmospheres. The corresponding K_p - V_{sys} maps are discussed in Section 4.7. Finally, Section 4.9 provides a summary and conclusion.

4.2 The iron signal of WASP-76b in high resolution

WASP-76b (West et al. 2016) is an archetypal ultra-hot Jupiter. With a semi-major axis of 0.033 AU, the planet orbits an F7-type main sequence star in 1.81 days. Recently, Ehrenreich et al. (2020) observed WASP-76b’s transit with VLT/ESPRESSO ($R = 138,000$) in both high *spectral* and *temporal* resolution, and claimed evidence for neutral iron (Fe I) condensation on its nightside. Transit observations provide valuable insights into the non-uniformity of ultra-hot Jupiters, because they probe the terminator region of the atmosphere. The terminator region constitutes the interface between the dayside and the nightside of the planet, and can thus be expected to feature extreme thermal and chemical gradients. Because WASP-76b resides so close to its host star, the planet rotates by no less than 30 degrees during its transit. In combination with the gradients throughout the atmosphere, this large angle must inevitably lead to changes in the transmission spectrum with time. Such changes can only be interpreted with 3D models.

As briefly discussed in Section 3.1.1, Ehrenreich et al. (2020) indeed reported a phase-dependence in the transmission spectrum of WASP-76b. Across the wavelength range covered by VLT/ESPRESSO (0.38–0.79 micron), gaseous iron is responsible for the most prominent absorption lines contained in the spectrum. In high spectral resolution, these lines are swamped by noise, so the spectrum must be multiplied with a template to obtain a cross-correlation function (CCF, see Section 2.3.3). The peak position of the CCF reveals the average radial velocity (RV) by which iron in the observable atmosphere is moving with respect to the observer. Fig. 4.1 shows the iron absorption signal that Ehrenreich et al. (2020) measured, along with the signal reported by Kesseli & Snellen (2021), who applied

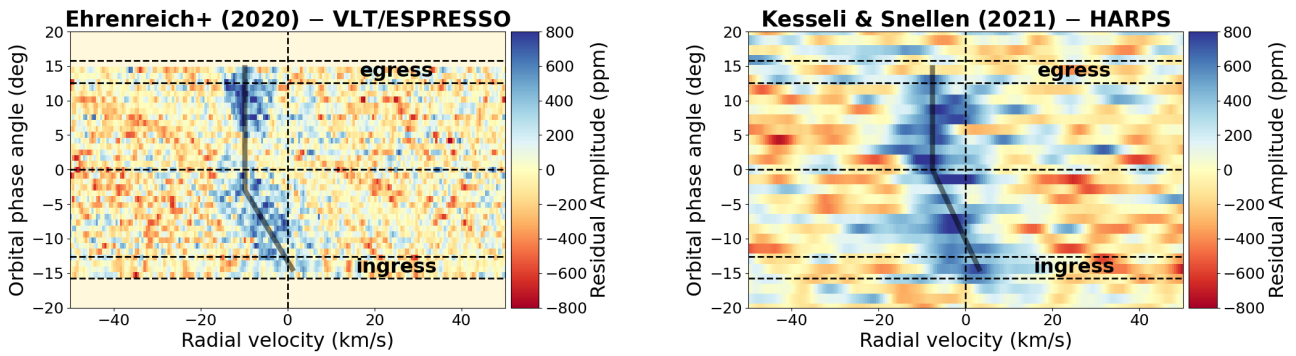


Figure 4.1: The asymmetric iron absorption signal of WASP-76b, as measured by Ehrenreich et al. (2020) and Kesseli & Snellen (2021). The observations were transformed to the planetary rest frame, to exclude contributions from orbital and systemic motion. The maps were obtained by cross-correlating the planetary spectra with templates containing iron lines. The signals indicate the average radial velocity by which gaseous iron (Fe I) in the observable atmosphere of WASP-76b is moving with respect to the rest frame. The solid black lines indicate the overall trends, but are by no means a fit to the data. The signal from Ehrenreich et al. (2020) fades between 0 and 5 degrees, due to an overlap between the Doppler shadow of the star and the planetary signal.

the same technique to HARPS data ($R = 115,000$; 0.38–0.69 micron) to independently confirm the phase-dependence of the observation. It should be noted that the signals in Fig. 4.1 pertain to the planetary rest frame, which moves with the planet as it orbits the star. In this frame, the CCF of a static atmosphere without winds and rotation will always have a peak at 0 km/s, because there is no moving material to Doppler shift the absorption lines. Although the measurements from Ehrenreich et al. (2020) and Kesseli & Snellen (2021) may differ slightly in terms of RV values, their qualitative behaviour is very similar. As illustrated in Fig. 4.1, the iron signal of WASP-76b lies close to 0 km/s at ingress, but the spectrum becomes progressively more blueshifted in the first half of the transit. Around mid-transit, the signal features a “kink”, after which the RV remains more or less constant. At egress, the Ehrenreich et al. (2020) signal is located at -11 km/s, while that of Kesseli & Snellen (2021) ends up near -8 km/s.

To explain the behaviour of the iron signal, Ehrenreich et al. (2020) suggested a combination of tidally locked rotation, day-to-night winds, an eastward hotspot shift, and (nightside) condensation of iron as an explanation for their observations. In the proposed scenario, the hotspot shift causes the leading limb to be cooler than the trailing limb¹. If the temperature on the leading limb is low enough, iron will condense out of the atmosphere, such that there is an asymmetric distribution of iron across the dayside.

Fig. 4.2 summarises what happens in this scenario. At ingress, the stellar light only penetrates the leading limb. Gaseous iron is carried by *blueshifting* day-to-night winds that counteract the *redshifting* planetary rotation. These contributions add up to a net Doppler shift of roughly zero. As the trailing limb moves in front of the star, the signal becomes more blueshifted. This is because the day-to-night flow and planetary rotation both move

¹In this work, the *trailing limb* will be synonymous for the evening terminator (or east limb). It is the part of the atmosphere that rotates away from the star and towards the observer. Likewise, we use the term *leading limb* to refer to the morning terminator (or west limb), which rotates towards the star and away from the observer (See Fig. 4.2). We are aware that some studies use more stringent definitions for the *limb* and the *terminator* (e.g., footnote 1 in Caldas et al. 2019).

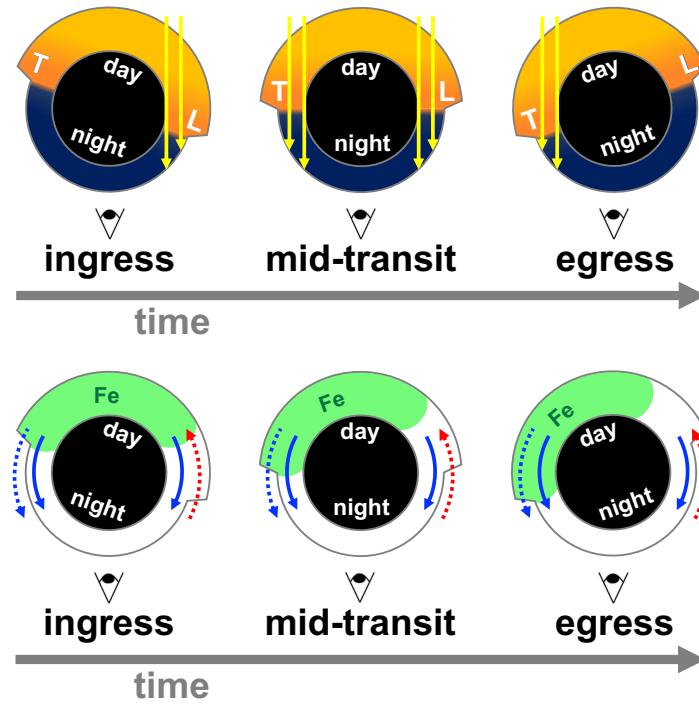


Figure 4.2: The equatorial plane of WASP-76b. **Top row:** The orientation of the planet at three stages during the transit. The yellow region denotes the hot dayside atmosphere and the blue region the cooler nightside. The outer contour of the images represents an isobar, which lies further from the center of the planet on the (puffy) dayside than on the (compact) nightside. The pairs of yellow arrows show stellar light rays crossing the atmosphere. The trailing and leading limb of the planet are labelled T and L, respectively. **Bottom row:** The iron (Fe I) distribution of WASP-76b as proposed by [Ehrenreich et al. \(2020\)](#). The green region on the dayside is abundant in iron, while the white region is depleted. Moreover, the solid arrows show the direction of day-to-night winds, while the dotted arrows indicate the direction of planetary rotation. Note that angles and sizes in the figure have been exaggerated for visualisation purposes.

iron towards the observer on this side of the planet. In the meanwhile, the signal from the leading limb becomes weaker as the amount of iron along the line of sight decreases. After mid-transit, the iron on the leading limb has rotated out of view completely and the signal dominated by the trailing limb.

WASP-76b is not the only ultra-hot Jupiter for which *phase-dependent iron absorption* has been reported in transmission. [Borsa et al. \(2021\)](#) observed WASP-121b with VLT/ESPRESSO and found a signal very similar to that of [Ehrenreich et al. \(2020\)](#) and [Kesseli & Snellen \(2021\)](#), with the iron lines shifting to bluer wavelengths during the transit. Earlier on, WASP-121b observations by [Bourrier et al. \(2020a\)](#) had already demonstrated that the average blueshift of iron is larger in the second half of the transit than in the first half (-6.6 vs -3.8 km/s). [Hoeijmakers et al. \(2020\)](#) studied iron absorption in the atmosphere of the planet MASCARA-2b/KELT-20b and measured a time variability in the signal *strength* of singly-ionised iron (Fe II). Furthermore, they found that the Fe I and Fe II signals were blueshifted by different amounts, in agreement with earlier observations by [Stangret et al. \(2020\)](#). This result could indicate that the absorption lines of both species probe different layers of the atmosphere, each with its own wind speed. In the meanwhile, [Nugroho et al. \(2020\)](#) reported possible signatures of atmospheric dynamics and 3D effects based on the

K_p - V_{sys} map (see Section 2.3.4) of MASCARA-2b/KELT-20b. [Rainer et al. \(2021\)](#) also constructed K_p - V_{sys} maps and even found evidence for changes *between* different transits of the planet. As for KELT-9b, the hottest ultra-hot Jupiter known to date, [Hoeijmakers et al. \(2019\)](#) did not find a significant Doppler shift in the absorption signal of iron. [Cauley et al. \(2019\)](#), however, did report time variability in the *width* of the absorption lines.

Although these observations pertain to just a small set of ultra-hot Jupiters, they already highlight the plethora of ways in which 3D effects can manifest themselves in the data.

4.3 Methods

4.3.1 Global circulation model

We use the SPARC/MITgcm global circulation model ([Showman et al. 2009](#)) to simulate the atmosphere of WASP-76b under the assumption of tidal locking. The model solves the primitive equations on a cubed-sphere grid and combines 3D atmospheric dynamics with non-grey radiative transfer. The SPARC/MITgcm has been applied to a variety of hot Jupiters ([Showman et al. 2009, 2015](#); [Fortney et al. 2010](#); [Parmentier et al. 2013, 2016, 2021](#); [Kataria et al. 2015, 2016](#); [Lewis et al. 2017](#); [Steinrueck et al. 2019, 2021](#)), as well as a number of ultra-hot Jupiters ([Parmentier et al. 2018](#); [Arcangeli et al. 2019](#); [Pluriel et al. 2020](#)). To date, however, the only *high-resolution* study that made use of the SPARC/MITgcm was performed by [Showman et al. \(2013\)](#). We note that [Fortney et al. \(2010\)](#) also calculated transmission spectra from 3D atmospheric models, but their work exclusively focused on low resolution.

Model setup

The setup of our simulations is fully identical to that of [Parmentier et al. \(2018\)](#) – see their Section 2 for more details. The atmosphere has 53 vertical layers, over which the pressure decreases from 200 bar to 2 μ bar. We use a grid resolution of C32, roughly equivalent to 128 cells in longitude and 64 cells in latitude. The models are evolved for 300 days, with time steps of 25 seconds. The final temperature profiles and wind maps are obtained by averaging over the last 100 days of the simulation. Also, we note that the SPARC/MITgcm does not have a self-consistent cloud formation scheme. Instead, it uses equilibrium condensation and gas-phase chemistry to compute the abundances of gaseous species. The effects of iron condensation are mimicked through “rainout”, where we consider all the iron-bearing gases and condensates from [Visscher et al. \(2010\)](#). Rainout means that a particular fraction of the gaseous iron is simply removed from cells where the temperature lies below the (pressure-dependent) condensation temperature of a particular iron-bearing condensate.

We model the atmosphere of WASP-76b under four different conditions, summarised in Table 6.1. All models have the same (solar) abundances, but they differ in terms of their drag timescale τ_{drag} . This is the time it takes for winds to lose a significant fraction of their kinetic energy as a result of drag forces ([Showman et al. 2013](#), [Parmentier & Crossfield 2018](#)). These drag forces could stem from processes such as turbulent mixing ([Li & Goodman 2010](#)), Lorentz-force braking of ionised winds in the planet’s magnetic field ([Perna et al. 2010a](#)) and Ohmic dissipation ([Perna et al. 2010b](#)). In the absence of drag forces ($\tau_{\text{drag}} \rightarrow \infty$), (ultra-)hot Jupiters develop a superrotating jet around their equator. However, when the drag timescale becomes shorter, winds are slowed down and jet formation is suppressed

Table 4.1: Overview of the four WASP-76b scenarios simulated with the SPARC/MITgcm.

Model	Drag timescale	TiO and VO opacities
No drag	∞	✓
Weak drag	10^5 s	✓
Strong drag	10^4 s	✓
No drag w/o TiO+VO	∞	×

(Komacek & Showman 2016; Komacek et al. 2017). In this regime, the atmospheric circulation pattern is dominated by day-to-night winds across the entire terminator. We consider atmospheres with τ_{drag} values of ∞ (no drag), 10^5 s (weak drag) and 10^4 s (strong drag), respectively.

Besides these three models, we also study a drag-free atmosphere where the opacities of TiO and VO are assumed to be zero, both in the GCM and in the post-processing (no drag w/o TiO+VO). Such a model mimics the effects of a “cold trap” (Spiegel et al. 2009; Parmentier et al. 2013; Beatty et al. 2017), where the nightside condensation of TiO and VO leads to cloud particles that settle gravitationally. If the vertical mixing in the atmosphere is not strong enough to carry these particles aloft again, the upper atmosphere will become depleted of TiO and VO, both on the dayside and the nightside of the planet. Normally, TiO and VO are important optical absorbers and act as thermal-inversion agents in the atmospheres of ultra-hot Jupiters (Hubeny et al. 2003; Fortney et al. 2008; Gandhi & Madhusudhan 2019). Hence, the presence of a cold trap should change the radiative feedbacks in the atmosphere, resulting in a different temperature structure and wind profile.

In this work, we do not examine the effects of departures from solar-composition abundances. As will be shown later in this chapter, our results are mainly driven by asymmetries between the trailing and the leading limb of the planet, and we do not expect these to change substantially as a function of metallicity or C/O ratio. A higher metallicity would shift the whole temperature structure of the atmosphere to lower pressures, while increasing the day-night contrast (Kataria et al. 2015). As for C/O, only Mendonça et al. (2018) studied the effect of the C/O ratio on the atmospheric circulation. We expect that small C/O variations will have a similar impact as changes in the metallicity, because for $\text{C/O} < 1$ the only optically important species to become more or less abundant is water (the amount of CO will also change, but is less important to the radiative transfer). To our knowledge, highly non-solar metallicities or C/O ratios larger than unity have not been unambiguously detected in exoplanet atmospheres, so we propose to leave the exploration of this part of parameter space for later work.

A note on previous studies

With regards to previous 3D modelling studies, it should be noted that the majority of recent works (Miller-Ricci Kempton & Rauscher 2012; Zhang et al. 2017; Flowers et al. 2019; Harada et al. 2021; Beltz et al. 2021) made use of the GCM from Rauscher & Menou (2012), which employs double-gray radiative transfer. This means that the GCM uses one opacity value κ_{vis} for shortwave (optical) radiation and another value κ_{ir} for longwave (infrared) radiation – thereby ignoring the more intricate wavelength-dependence of the atmospheric opacities. One of the downsides of this approach is that the model tends to produce isothermal tem-

perature profiles above the photosphere (Parmentier & Guillot 2014), where the atmosphere neither absorbs nor emits a significant amount of radiation. That said, it is hard to judge to what extent high-resolution transmission spectra “suffer” from the double-gray approximation. Kempton et al. (2014) demonstrated for a suite of hot Jupiters that absorption features are hardly sensitive to the precise *vertical* shape (e.g. inversions) of the temperature structure, which suggests that isothermal profiles may not be problematic in transmission², as long as *longitudinal* variations are properly captured.

The SPARC/MITgcm, employed in this work, uses non-grey radiative transfer to evaluate its heating and cooling rates, resulting in quantitatively different temperature structures and perhaps different 3D wind profiles (Showman et al. 2013). However, no detailed comparison between the SPARC/MITgcm and the GCM from Rauscher & Menou (2012) has ever been carried out. Also, there will be more differences between both models besides their radiative-transfer treatment, and this makes it hard to interpret any disagreement between their outputs. For example, Miller-Ricci Kempton & Rauscher (2012) and Showman et al. (2013) both performed simulations of HD 209458b and found different wind speeds in cases where they did not include drag forces. To our knowledge, the precise origin of the discrepancies has never been investigated.

4.3.2 Mapping GCM outputs onto a spherical grid

The GCM uses pressure as a vertical coordinate. However, in the context of optical depths and transit spectra, we are actually interested in physical distances along the line of sight. Therefore, the GCM atmospheres need to be mapped onto a spherical grid with altitude as a vertical coordinate. Because the atmospheres have a different temperature profile in each atmospheric column (with latitude α and longitude φ), grid points at the same pressure level P do not correspond to the same altitude z .

For each latitude and longitude, we calculate the heights associated with the cell centres $\{z\}$ and the cell boundaries $\{\bar{z}\}$:

$$\begin{aligned} z_i &= \bar{z}_i + H \ln(\bar{P}_i / P_i) \\ \bar{z}_{i+1} &= \bar{z}_i + H \ln(\bar{P}_i / \bar{P}_{i+1}) \end{aligned} \quad (4.1)$$

In these equations, symbols with bars are defined on the cell boundaries and those without bars in the cell centres, where it holds that $P_i < \bar{P}_i$. The lower boundary of the bottom cells coincides with the bottom of the atmosphere, such that $\bar{z}_1 = 0$ and $\bar{P}_1 = 200$ bar. The scale height follows from $H = P_i / \rho_i g$, with ρ_i the local density. The gravity³ is given by $g = GM / (R_0 + \bar{z}_i)^2$, with M the mass of the planet and R_0 its radius at the bottom of the atmosphere. Once the heights of the cell centres are known, we interpolate the GCM output onto a spherical grid with coordinates (α, φ, z) , where $\alpha \in [-90^\circ, 90^\circ]$ is the latitude, $\varphi \in [-180^\circ, 180^\circ]$ is the longitude, and z is the altitude.

As depicted schematically in Fig. 4.2, the daysides of our models have a substantially larger scale height than the nightsides, owing to the vast temperature difference between both hemispheres. In the strong-drag model, for instance, the atmospheric column that runs

²The vertical shape of the temperature structure does have a big impact on high-resolution *emission* spectra. For instance, when the atmosphere is isothermal, the emission spectrum will have no features because the core-to-continuum contrast is zero.

³In the GCM, a constant gravity $g = GM / R_0^2$ is assumed at all pressures.

from 200 bar to 2 μ bar at the substellar point is a factor ~ 2.3 taller than at the anti-stellar point. Because the spherical grid goes up to the same altitude everywhere, we are forced to extrapolate the nightsides down to lower pressures, such that the atmosphere is specified at each grid point. To this end, we assume that all cells above the GCM boundary (at 2 μ bar) have temperatures, chemical abundances and wind speeds equal to those in the highest cell *below* the GCM boundary. Densities follow from $\rho_i = P_i / RT_i$, with R the specific gas constant of the atmosphere. We verified that the precise extrapolation assumptions have little effect on the final cross-correlation signals, since the bulk of the absorption occurs at the higher pressures within the GCM boundary (that is, within our selected wavelength windows – see Section 4.3.3).

Another point should be made regarding the wind vectors. In the GCM, the components of the wind vectors are defined as being tangent and orthogonal to isobaric surfaces. However, this is no longer the case once the GCM output has been mapped onto (α, φ, z) coordinates. Especially in regions where a large temperature gradient occurs (around the terminator), there will be an angle γ between the local isobaric surface and the surface of equal altitude. On numerical grounds, however, we expect the impact of this anomaly to be small in relation to the final cross-correlation signals. That is, for all atmospheres, we find that $\gamma \lesssim 20^\circ$ in the cells adjacent to the terminator plane⁴. The projection factor associated with this angle is $\cos(\gamma) \approx 0.94$, which means that the line-of-sight wind speeds may be off by at most $\sim 6\%$ in those cells. In practice, the absorption always takes place in multiple cells along a transit chord (some further away from the terminator plane), so the overall error in the Doppler shifts due to winds will be smaller than this value.

4.3.3 Modelling the transit of WASP-76b

Computing spectra

We use HIRES-MCRT (the predecessor of gCMCRT) to compute self-consistent transmission spectra of the four WASP-76b models (see Section 4.3.1) at 37 orbital phases during the transit. Once mapped onto the spherical grid, the atmospheres have a radius $R = R_0 + z_{\max} \approx 2.2R_{\text{Jup}}$, with the 1-bar surface situated between 1.8 and 1.9 R_{Jup} . Additionally, the semi-major axis of the planet’s orbit is 0.033 AU. Combined with the radius of the host star, $R_\star = 1.73R_\odot$, this means that the ingress starts at $\phi \approx -15.6^\circ$ (first contact) and ends at $\phi \approx -12.1^\circ$ (second contact). Hence, assuming that the system is viewed exactly edge-on, the full transit subtends $\sim 31^\circ$. Since WASP-76b is tidally locked, this is also the angle by which the atmosphere rotates during the observation. In the ingress and the egress phase, we only illuminate those regions of the atmospheric annulus that are blocking the star.

Transmission spectra are computed in two narrow windows (364.5–367.6 nm and 378.5–381.7 nm) at $R = 500,000$, which contain 3617 and 4210 wavelength points, respectively. The cross sections of Fe I in these two windows are plotted in Fig. 4.3. In the first wavelength window, the opacity is mainly comprised of weak lines that show a considerable temperature-dependence. On the other hand, the second window includes a number of strong lines with broad wings and a fairly constant strength. Because we do not suffer from physical noise in our model, we can afford to limit our study to only a couple of thousand wavelength points for the sake of computational feasibility. In reality, observations require

⁴For the drag-free model without TiO and VO opacities, we find $\gamma \lesssim 10^\circ$

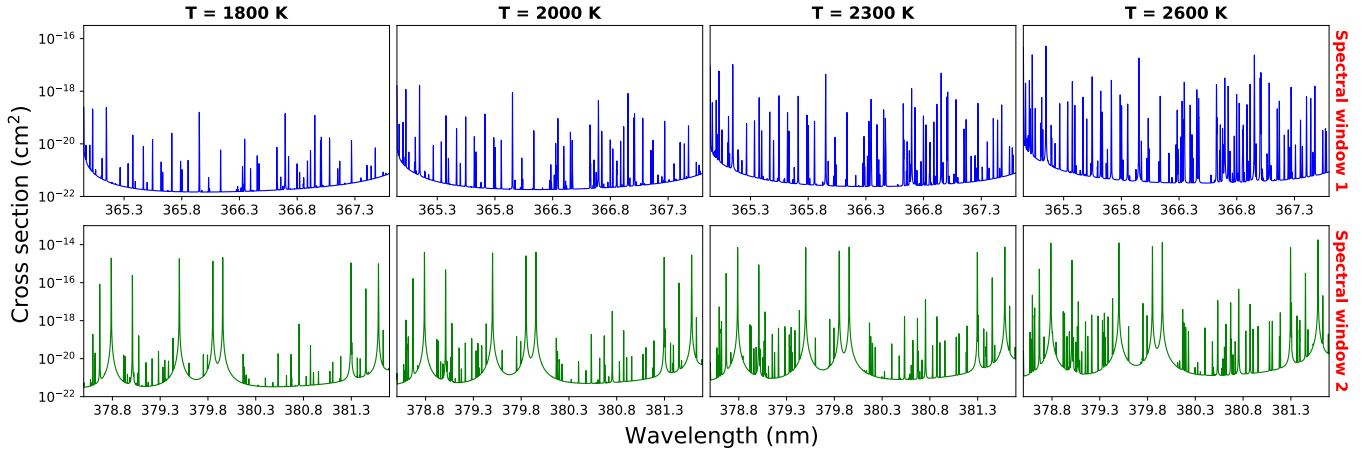


Figure 4.3: The cross-sections of neutral iron (Fe I) at a pressure of 0.3 mbar and four different temperatures (columns). The cross-sections are shown in two wavelength windows (rows), both of which are used to simulate spectra in this work. The top row (window 1) mainly contains weak lines, while the bottom row (window 2) comprises a number of strong lines with broader wings.

a much larger set of absorption lines to achieve a sufficiently strong signal. This is because the planetary spectrum is typically buried in (stellar) noise.

In HIRES-MCRT, we account for the cross-sections of Fe I (Kurucz & Bell 1995), Na (Allard et al. 2003), K (Allard et al. 2016), VO, TiO, and opacities due to bound-free and free-free transitions associated with H^- (John 1988). The absorption cross-sections of the metal oxides, TiO and VO, are from the EXOPLINES database (Gharib-Nezhad et al. 2021a)⁵ and were generated by Gharib-Nezhad et al. (2021b), using line lists including ExoMol (Tennyson et al. 2020) and MoLLIST (Bernath 2020).

The rationale behind modelling spectra in *two* wavelength windows is the fact that lines of different strength probe the atmosphere at different depths. Hence, spectra in different wavelength windows may be sensitive wind speeds in different regions of the atmosphere. To verify that our simulations are more or less representative of the entire wavelength range spanned by the observations (Ehrenreich et al. 2020; Kesseli & Snellen 2021), we computed the CCFs for both windows separately and compared the resulting signals. In spite of some numerical discrepancies, the same trends could be recovered, suggesting that our analysis is at least qualitatively robust. Furthermore, all CCF maps shown in this chapter (see Sections 4.5 and 4.6) are obtained by *adding* the maps of both wavelength windows together – analogous to combining the signals from different spectral orders in real observations (e.g., Nugroho et al. 2021).

We note that the opacities of TiO and VO become stronger with increasing wavelength throughout the ESPRESSO and HARPS orders. Hence, if TiO and VO are present in the (observable) atmosphere, the weak iron lines towards the redder end of the spectrum may have reduced amplitudes, which causes the observed CCF signal to be more sensitive to the iron lines in the blue part of the spectrum (simulated in this work). Spectra of an atmosphere *without* TiO and VO do not suffer from this muting effect and may thus contain more weak iron lines at longer wavelengths. We recognise that the models presented in this work do not account for differences in muting or aliasing between models with and without TiO/VO, and this requires more attention in future studies.

⁵[Link to EXOPLINES opacity data](#)

Computing cross-correlations

To compute cross-correlation maps of the simulated observations, we use the spectrum of the *static*⁶ atmosphere at mid-transit as our template $\vec{T}$ (see equation 2.39). Prior to multiplying the template with the spectra at each of the 37 orbital phases, we subtract its mean such that

$$\sum_{j=1}^{N_\lambda} T_j = 0. \quad (4.2)$$

As a result, the template is not sensitive to (constant) offsets in the spectrum, but only to the strength of the spectral features relative to a horizontal baseline. That is,

$$\text{CCF} = \sum_{j=1}^{N_\lambda} (x_j + c) T_j = \sum_{j=1}^{N_\lambda} x_j T_j + c \sum_{j=1}^{N_\lambda} T_j = \sum_{j=1}^{N_\lambda} x_j T_j, \quad (4.3)$$

with c a constant.

Additionally, we calculate the K_p - V_{sys} maps based on the 29 *in-transit* spectra, so we ignore the ingress and egress phase. This prevents us from having to deal with limb sectors that are only partially illuminated by the star, which complicates the treatment.

4.4 GCM structures and transmission spectra

4.4.1 Four atmospheric models of WASP-76b

Fig. 4.4 shows the temperatures and iron abundances in the equatorial plane of the WASP-76b models obtained from the GCM. As mentioned previously, the dayside is substantially more extended than the nightside, due to the large temperature contrast between both hemispheres. It can be seen that the nightside of the drag-free atmospheres is slightly warmer (especially between 10 and 0.1 bar) compared to the models with drag, owing to more efficient heat redistribution. Furthermore, the dayside of the first three models features a strong thermal inversion between 0.1 and 10^{-3} bar, where the temperature increases with altitude. The plots also reveal a hotspot shift, a displacement of the hottest region away from the sub-stellar point. In the drag-free scenarios, the atmospheric layers between 0.1 and 10^{-3} bar are hotter to the east of the sub-stellar point than to the west. However, as the drag timescale becomes shorter, the hotspot shift diminishes – a result that is in agreement with the literature (Showman & Polvani 2011, Parmentier & Crossfield 2018, Tan & Komacek 2019).

Because the drag-free model without TiO and VO opacities lacks important optical absorbers, its temperature structure is qualitatively different from that of the other models. In particular, its hotspot offset extends to much lower pressures $\sim 10^{-4}$ bar, resulting in a larger asymmetry between the trailing and leading limb of the planet. As shown in the right panels of Fig. 4.4, the day-night transition to smaller scale heights appears to be more gradual on the leading limb than on the trailing limb. The atmosphere also has a steep thermal inversion on its dayside, but it occurs higher up in the atmosphere compared to the other models, at pressures below 10^{-3} bar. This inversion is likely due to sodium absorption in the upper atmosphere.

⁶In the *static* models, we set $v_{\text{los}} = 0$ km/s in all cells.

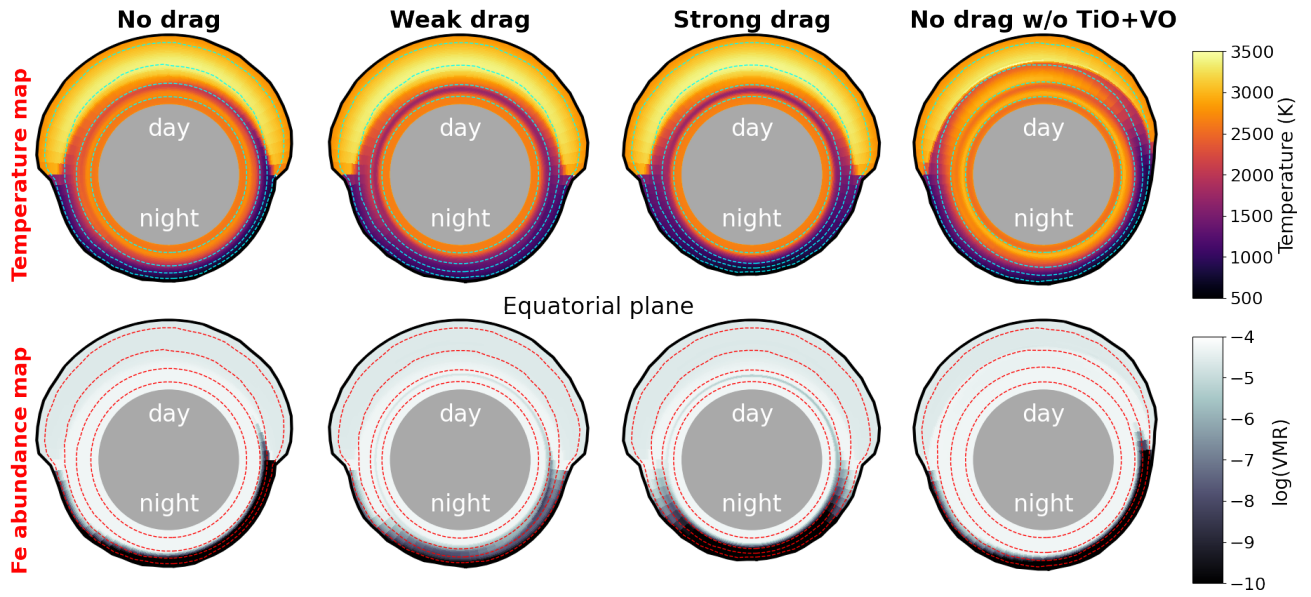


Figure 4.4: **Top row:** Temperatures in the equatorial plane of the of the four GCM atmospheres listed in Table 6.1. The maps are plotted as a function of spatial coordinate, with the dashed lines denoting isobars of 10^1 , 10^{-1} , 10^{-3} and 10^{-5} bar, respectively. The solid black contour marks the GCM boundary at $2 \mu\text{bar}$. **Bottom row:** Iron abundances in the equatorial plane, expressed in terms of volume mixing ratio (VMR). Note that the size of the atmosphere with respect to the rest of the planet has been enhanced for visualisation purposes.

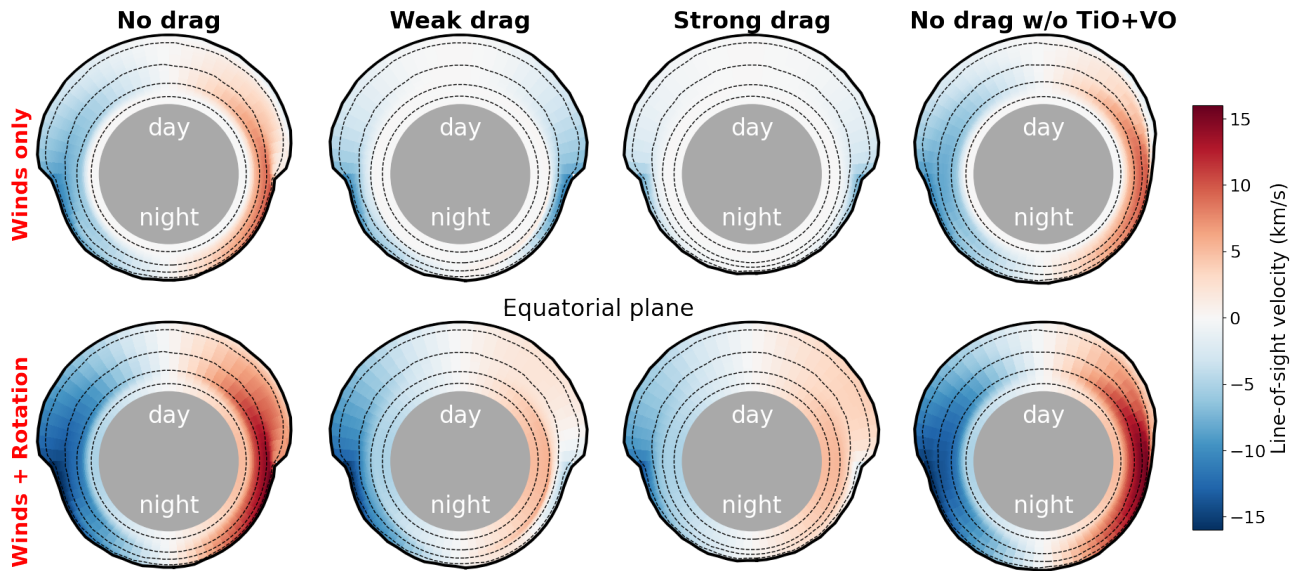


Figure 4.5: **Top row:** Line-of-sight velocities due to winds in the equatorial plane of the of the four GCM atmospheres listed in Table 6.1. A redshift (blueshift) indicates that the winds are blowing away from (towards) the observer. The maps are plotted as a function of spatial coordinate, with the dashed lines denoting isobars of 10^1 , 10^{-1} , 10^{-3} and 10^{-5} bar, respectively. The solid black contour marks the GCM boundary at $2 \mu\text{bar}$. **Bottom row:** The same plots, but with the contribution from planetary rotation added.

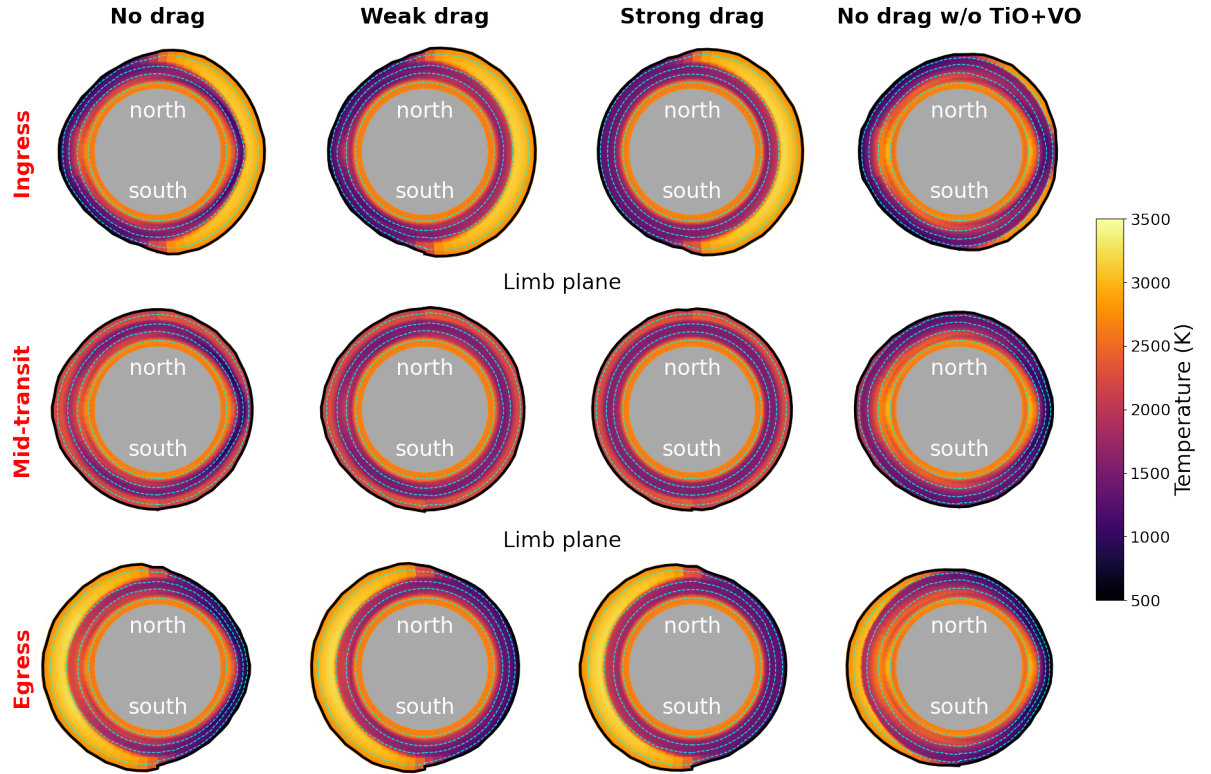


Figure 4.6: Temperatures in the limb plane of the four GCM models (columns), at different phases during the transit (rows). The maps are plotted as a function of spatial coordinate, with the dashed lines denoting isobars of 10^1 , 10^{-1} , 10^{-3} and 10^{-5} bar, respectively. The solid black contour marks the GCM boundary at $2 \mu\text{bar}$.

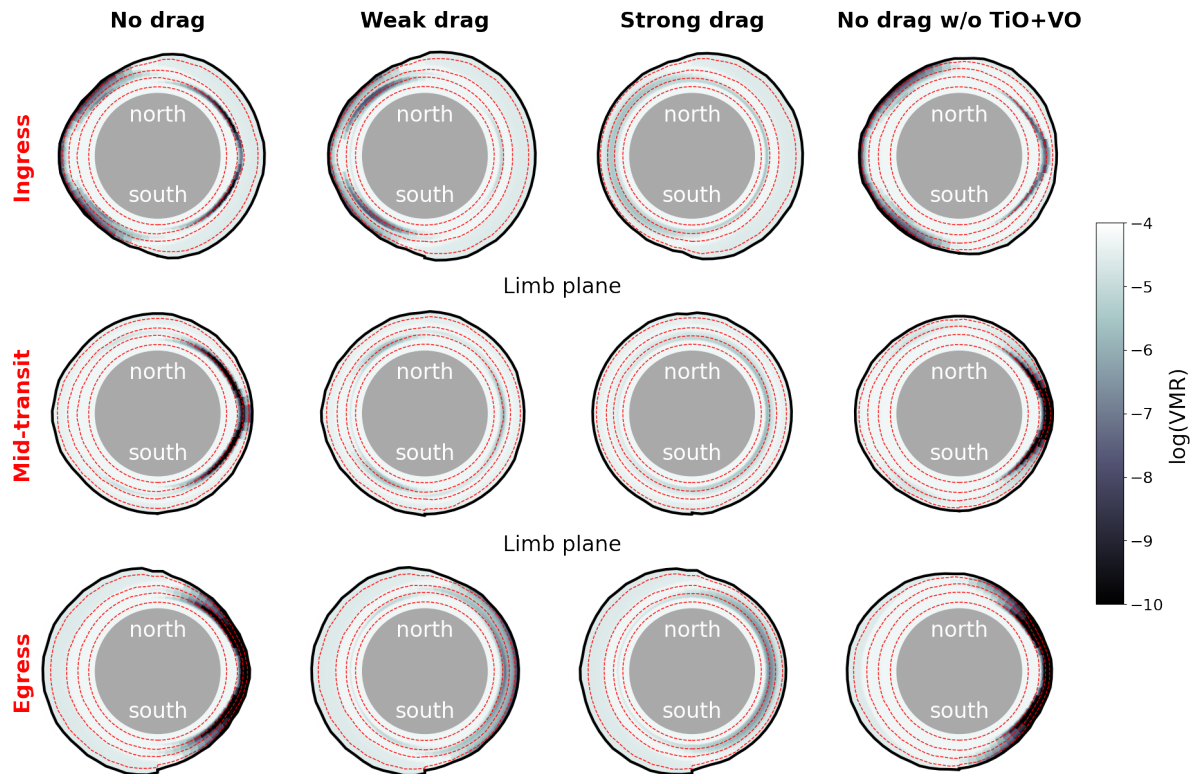


Figure 4.7: Same as Fig. 4.6, but now for the iron (Fe I) abundances.

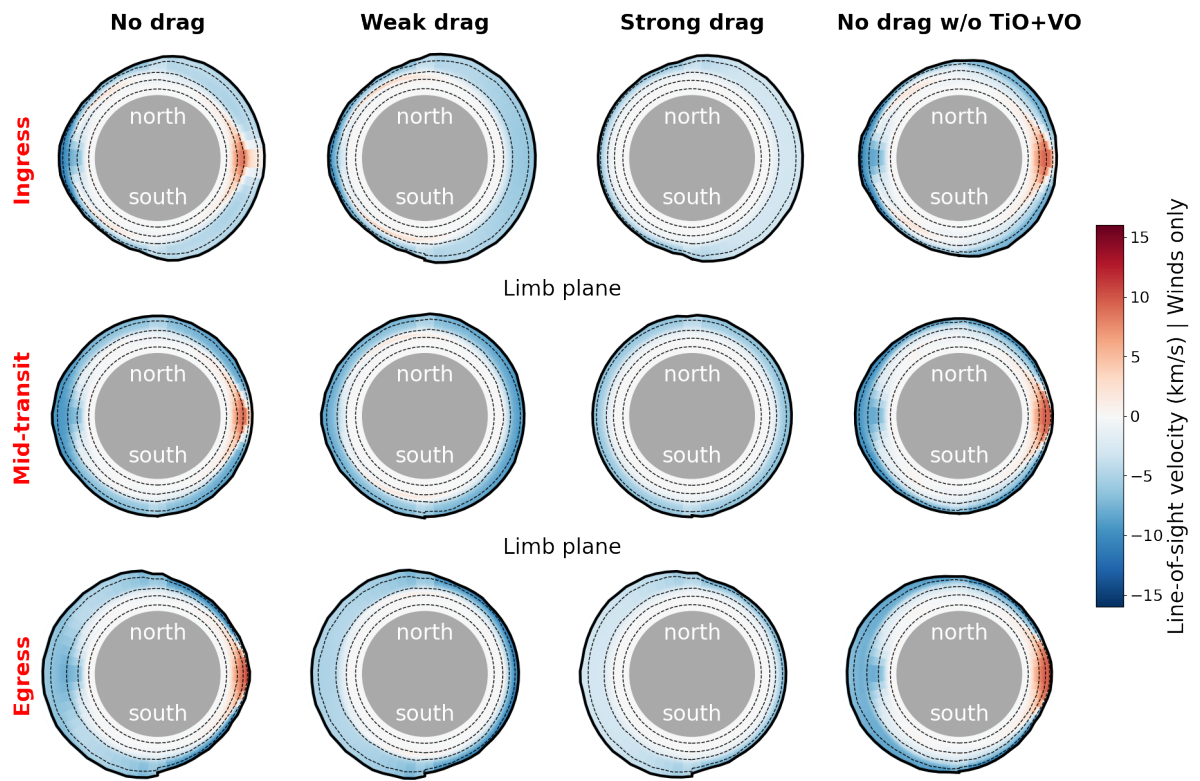


Figure 4.8: Same as Fig. 4.6, but now for the line-of-sight velocity due to winds only.

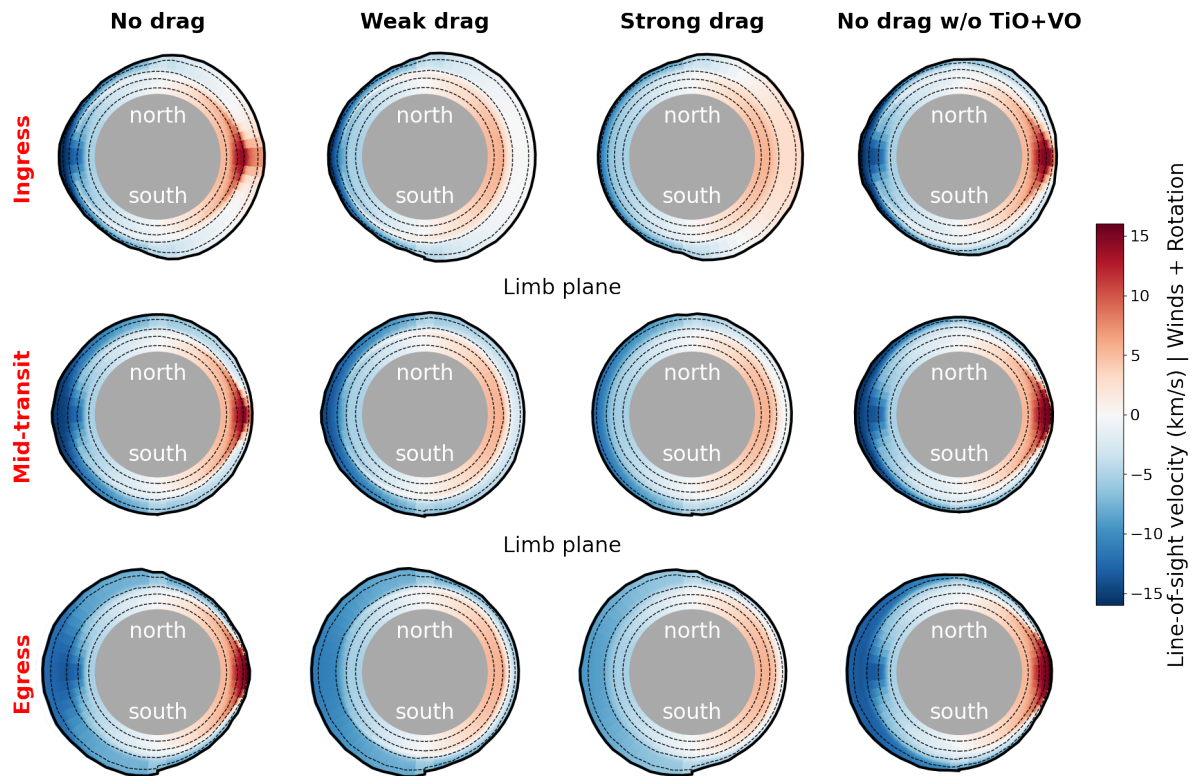


Figure 4.9: Same as Fig. 4.6, but now for the line-of-sight velocity due to winds and planetary rotation.

As far as chemistry is concerned, the bottom panels in Fig. 4.4 illustrate that iron is more or less uniformly distributed over the dayside of the WASP-76b models. On the cooler nightside, however, the upper regions of the atmosphere are (almost) fully depleted of iron as a result of condensation. As discussed in Section 4.3.1, the GCM accounts for condensation through rainout.

Fig. 4.5 shows the line-of-sight velocities of the atmospheres in the equatorial plane. We distinguish between the line-of-sight velocities due to winds only (top rows) and those due to the combined effect of winds and rotation (bottom rows). A number of things can be pointed out. Firstly, the models without drag develop an eastward equatorial jet. As a consequence, the associated line-of-sight velocities are negative on the trailing limb and positive on the leading limb. When drag forces are introduced, both limbs become blueshifted as jet formation around the equator is inhibited. Also, the shorter the drag timescale becomes, the lower resulting the wind speeds.

When planetary rotation enters the equation, the atmosphere's trailing limb (which rotates towards the observer) picks up an additional blueshift, while the leading limb (which rotates away from the observer) acquires a redshift. It should be noted that the contribution from rotation to the line-of-sight velocities is greatest in the equatorial regions, which lie furthest away from the rotation axis. Around the equator, the rotational velocity of WASP-76b is ± 5.3 km/s. At the poles, the contribution is zero.

In Figs. 4.6–4.9, we visualise the limb plane of the four GCM models. The plots depict the temperature, iron abundances, and line-of-sight velocities of the planet at *three different phase angles* encompassed by the transit: ingress ($\phi = -14^\circ$), mid-transit ($\phi = 0^\circ$) and egress ($\phi = +14^\circ$). By definition, the limb plane crosses the centre of the planet and is orthogonal to the line of sight. It coincides with the terminator plane at mid-transit. The plot demonstrates how the projected shape of the planet changes over time, as the dayside rotates out of view on the leading limb and into view on the trailing limb. Furthermore, in the models without drag, it can be seen that the extent of the equatorial jet is relatively small. The majority of the limb plane is blueshifted by day-to-night winds.

4.4.2 Transmission spectra

Fig. 4.10 shows a number spectra computed with HIRES-MCRT (for the drag-free and weak-drag atmospheres), in a small section of the first wavelength window. We distinguish between spectra that only include Doppler shifts due to winds (first three terms in equation 2.5), and spectra including the effects of both winds and planetary rotation (all terms in equation 2.5). A number of things can be pointed out. Firstly, all spectra are blueshifted by several km/s compared to the spectrum of the static atmosphere (with $v_{\text{LOS}} = 0$ km/s everywhere). Also, the absorption lines in the wind-only spectra are slightly broadened due to a dispersion in the (line-of-sight) wind speeds across the atmospheric limb. Planetary rotation further broadens the absorption features, as opposite redshift and blueshift contributions tend to pull the lines apart. Finally, Fig. 4.10 demonstrates that the spectra at $\phi = -10.5^\circ$ are different from those at $\phi = +10.5^\circ$. The shapes, positions and depths of the lines change during the transit, and this is a direct effect of the 3D geometry of the observation – different parts of the atmosphere are probed at different orbital phases, resulting in a phase-dependent signal.

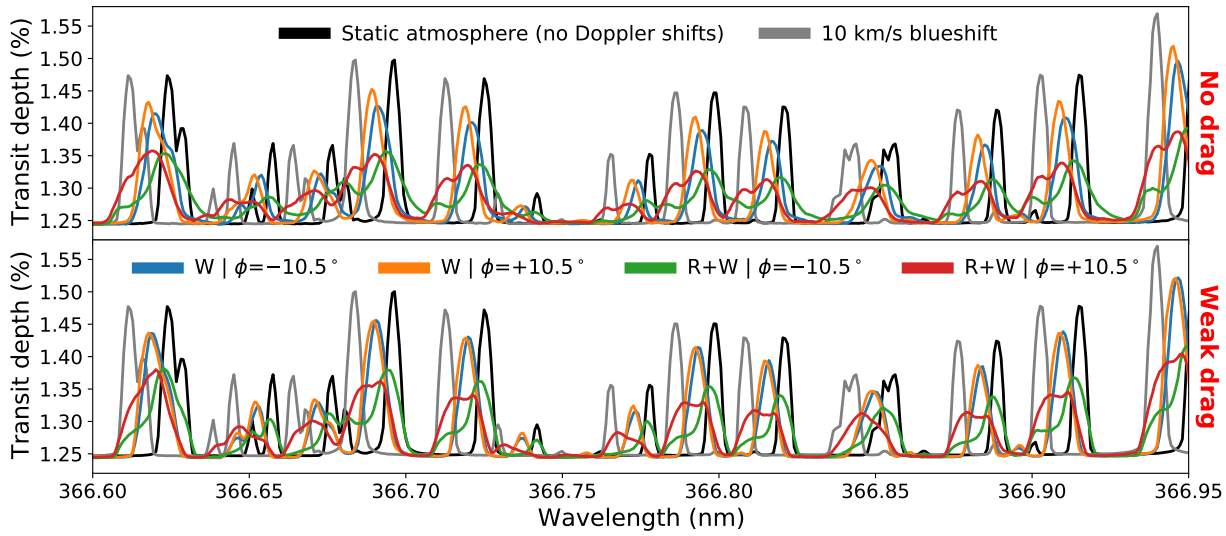


Figure 4.10: Transmission spectra of the drag-free (top panel) and the weak-drag (bottom panel) atmospheres, at phase angles -10.5° and $+10.5^\circ$. For both orbital phases, two spectra are plotted: one (W) that only includes Doppler shifts due to winds, and one (R+W) that includes both the effects of winds and rotation. The spectrum of the static atmosphere, with $v_{\text{LOS}} = 0$ km/s in all cells, is plotted in the background. As a reference, the figure also shows the static spectrum offset by -10 km/s.

4.5 CCF maps of the weak-drag model

Since [Ehrenreich et al. \(2020\)](#) suggested that the atmosphere of WASP-76b only features day-to-night winds (and no equatorial jet), we start by examining the CCF maps of our weak-drag model, with $\tau_{\text{drag}} = 10^5$ s. In this section, we aim to interpret the structure of the maps and characterise the behaviour of the signals arising from different limb sectors.

4.5.1 Weak drag: the nominal model

The top row of Fig. 4.11 displays the CCF maps obtained for the weak-drag model of WASP-76b, where we account for Doppler shifts due to winds and planetary rotation. The top-right panel shows the signal corresponding to the full limb (observable in reality). Its maximum shifts from -1 km/s at the end of ingress to -5.5 km/s at the start of egress. In addition to the *location* of the CCF peak, the full width at half maximum (FWHM) and the normalised peak height (signal strength) also change over time, as illustrated in the bottom panels of Fig. 4.11. It should be noted that these quantities were computed after the subtraction of single baseline value from the entire CCF map.

It is no surprise that the planet’s cross-correlation map is phase-dependent. Because the planet rotates by ~ 30 degrees during its transit, the observation really probes different parts of the atmosphere at different orbital phases – especially around the equator. Furthermore, the polar regions, which are situated close to the rotation axis, are probed under different angles over time. This means we can expect the observation to be sensitive to spatial variations in the planet’s temperature and abundance maps, as well as to the magnitude and orientation of the wind profile.

To better understand the structure of the CCF map associated with the full limb, we

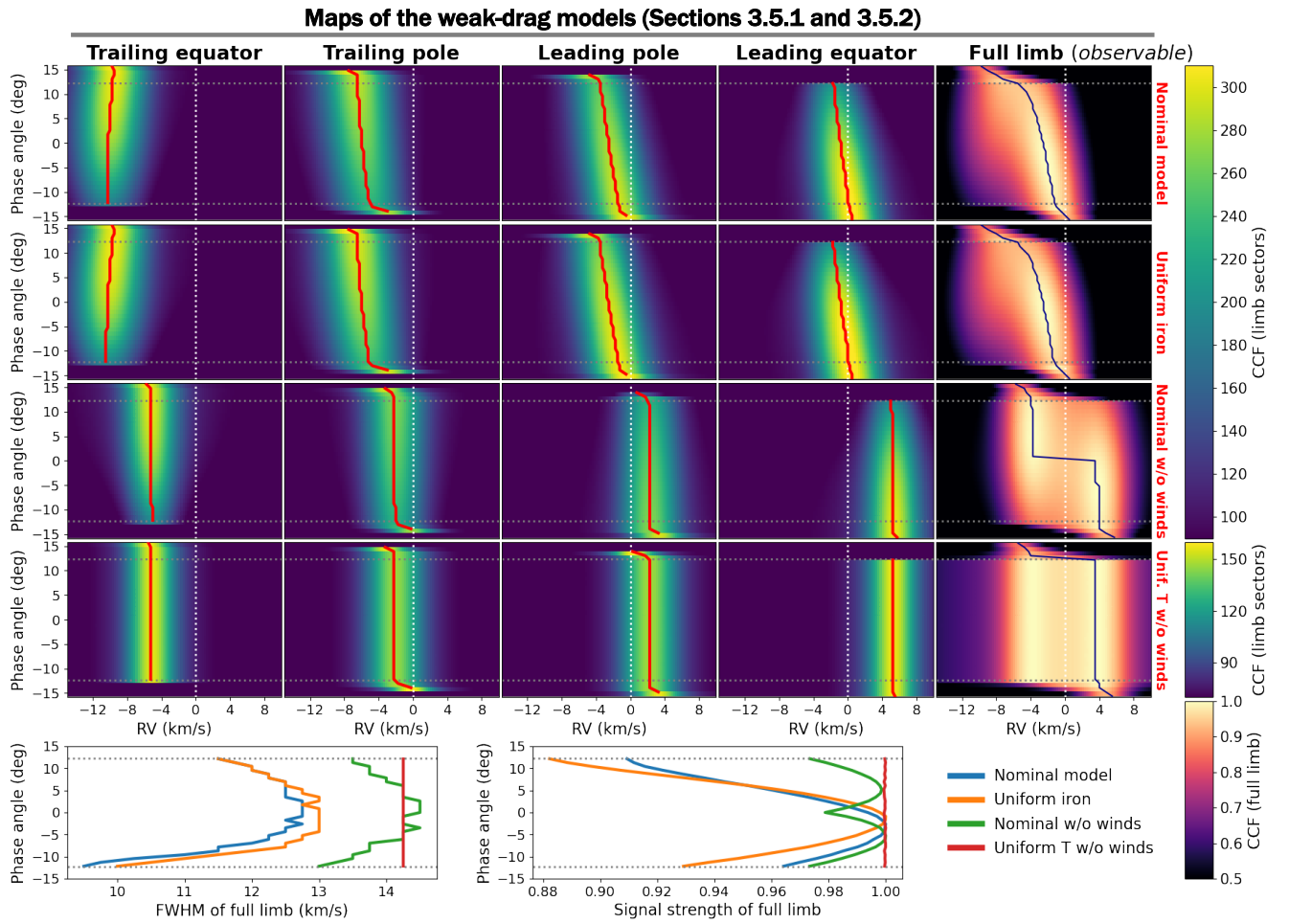


Figure 4.11: Top four rows: CCF maps of four atmospheres, all based on the weak-drag model from the GCM. The “nominal” model (top row) is the weak-drag model with Doppler shifts due to winds and rotation. The other atmospheres were obtained by making simple, ad hoc changes to the structure of the weak-drag model (see text). The first four columns pertain to the different limb sectors of the atmospheric annulus (see Fig. 2.2), while the right column shows the CCF maps of the full limb, normalised such that their maximum value is unity. Red and dark blue curves indicate the maxima of each map as a function of orbital phase. The horizontal dotted lines mark the end of the ingress and the start of the egress, respectively. **Bottom-left panel:** FWHM of the CCF maps of the full limb as a function of orbital phase. **Bottom-right panel:** Maxima of the CCF maps of the full limb as a function of orbital phase.

consider the CCF maps arising from each of the four limb sectors depicted in Fig. 2.2 – the trailing equator, the trailing pole, the leading pole and the leading equator. As demonstrated in Section 2.3.3, the CCF map of the full limb is simply the average of the (less complicated) CCF maps of the individual sectors. Hence, Fig. 4.11 allows us to interpret the different contributions to the overall signal separately, and link them to specific regions in the atmosphere.

The first thing to note is that each of the limb sectors has a different RV offset from the planetary rest frame. Moving from the left to the right panel in the first row of Fig. 4.11, one can see that the RV of the sectors becomes less negative. This trend is a direct effect of planetary rotation, which induces a blueshift on the trailing limb and a redshift on the leading limb. Also, the further away a sector from the rotation axis, the larger the magnitude of the

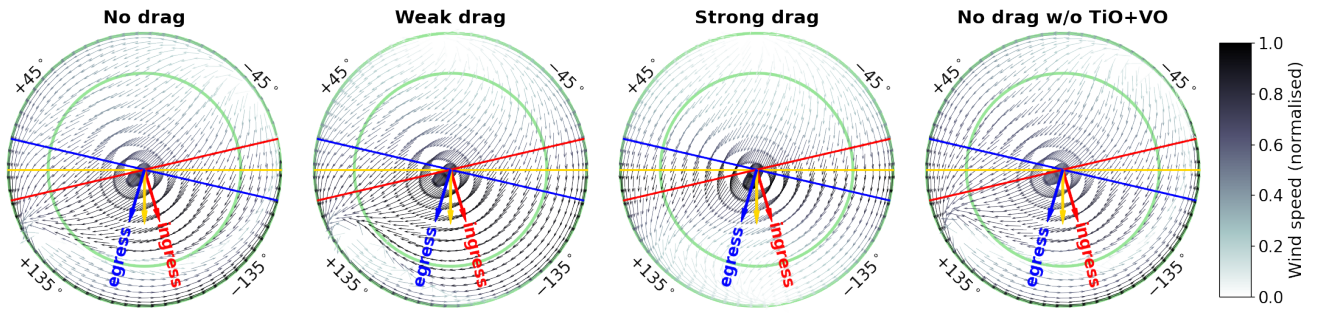


Figure 4.12: Wind profiles (at $P = 0.15$ mbar) of the four GCM models from Table 6.1, projected onto their northern hemisphere. We are looking down onto the planet from a point above its north pole. Each of the profiles is normalised to its own maximum. The darker the colour of the vectors, the higher the associated wind speeds. The green circles denote 0 and 45 degrees latitude. The solid lines represent the planet’s limb plane at ingress (red), mid-transit (yellow) and egress (blue), respectively. The plots demonstrate that the angle between the polar wind vectors and the line of sight (coloured arrow perpendicular to the limb plane) becomes smaller as the planet rotates from ingress to egress.

Doppler shift associated with rotation. Besides rotation, day-to-night winds also contribute to the RV offset, which is why all sectors are blueshifted.

The *slopes* in the RV signals of the sectors are due to the planet’s wind profile. On the trailing limb, the signal becomes marginally more redshifted with time, while the other sectors show an increasing blueshift with time. Around the poles, where roughly the same regions are probed during the transit, we are likely witnessing a projection effect. This is illustrated in Fig. 4.12. As the planet rotates between ingress and egress, the angle between the polar wind vectors and the line of sight becomes smaller, resulting in a more negative line-of-sight velocity with orbital phase. Near the equator, atmospheric regions move into and out of view faster, so the observation could actually probe different wind speeds there.

Besides the slopes and offsets of the RV shifts, the *signal strengths* also change in every sector – most noticeably around the equator. On the trailing equator, for instance, the CCF peak height increases during the transit. Fig. 4.2 illustrates why such behaviour is inherent to the atmospheres of ultra-hot Jupiters. Just after the ingress, when stellar light first crosses the trailing equator of the planet, the observation probes a relatively large part of the nightside (top left panel in Fig. 4.2). Yet, as the transit progresses, a larger part of the dayside rotates into view and the absorption takes place in progressively hotter regions. This has two consequences for the spectrum of the trailing equator, as demonstrated in Fig. 4.13: (i) the baseline moves up as the dayside is more puffy, and (ii) the absorption lines become stronger relative to the baseline. The reason for these stronger absorption lines is again twofold. Firstly, the weak iron lines become stronger with increasing temperature (see Fig. 4.3). Secondly, the scale height is larger in the hotter parts of the atmosphere, which results in bigger transit-depth variations with wavelength. In addition, the strong iron lines (one of which is shown in Fig. 4.13) acquire broader wings. Because the CCF is sensitive to line strength, its value must increase during the transit. The exact opposite occurs on the leading equator, which initially comprises a substantial part of the hot dayside. However, over the course of time, the nightside rotates into view and the absorption takes place in cooler regions with a smaller scale height. Similar effects occur around the poles, but the variations are less extreme, as the sectors are closer to the planet’s rotation axis.

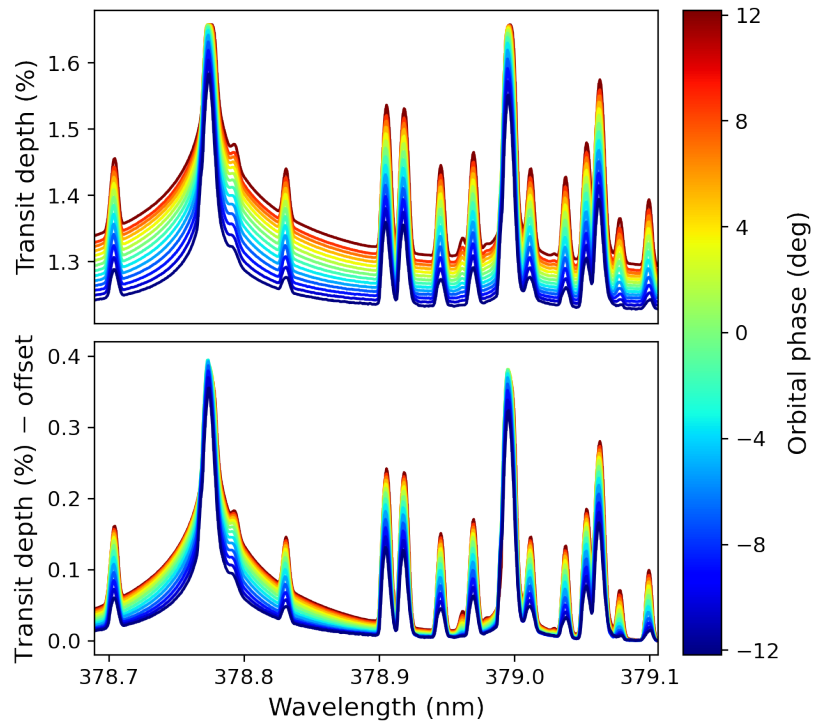


Figure 4.13: **Top:** Trailing-equator spectra of the weak-drag atmosphere (nominal model in Fig. 4.11) in a small section of the simulated wavelength range. The colour scale indicates different orbital phase angles. **Bottom:** The same spectra, but with their baselines subtracted.

4.5.2 Weak drag: variations on the nominal model

To further assess the impact of different atmospheric components, we apply simple modifications to the weak-drag model (i.e. the “nominal” model in Fig. 4.11) to see how the CCF maps of the planet change as a result of these modifications.

In the second row of Fig. 4.11, we set the iron abundances to $\log(\text{VMR}) = -4.3$ throughout the entire atmosphere. This scenario mimics an atmosphere where iron is uniformly distributed (in terms of VMR) and where no condensation takes place on the nightside, regardless of the temperature. As demonstrated in Fig. 4.11, the CCF maps of the uniform-iron model are very similar to those of the nominal model. This implies that the signal of the full limb reveals virtually nothing about the exact distribution of iron across the atmosphere. That is, we cannot differentiate between a model with uniform abundances and a model with iron abundances that follow from chemical equilibrium. The CCF maps of the nominal model do not serve as a proof for iron condensation on the nightside of the planet.

In the third row of Fig. 4.11, we set all winds to zero, such that the only contribution to the Doppler shift comes from planetary rotation. The RV shifts of the individual sectors are constant during the transit (excluding ingress and egress), but the heights of the CCF peaks still change over time. This proves that the varying signal strength is *not* an effect of atmospheric dynamics. As a result of the constant RV shifts in every sector, the CCF map of the full limb clearly features two modes. Both modes compete for the global maximum, which initially lies at positive RV. Halfway through the transit, however, it jumps to negative RV, owing to the fact that the signal strengths of the sectors change over time.

In the fourth row of Fig. 4.11, we set $T = 2300$ K in all cells and we use constant abun-

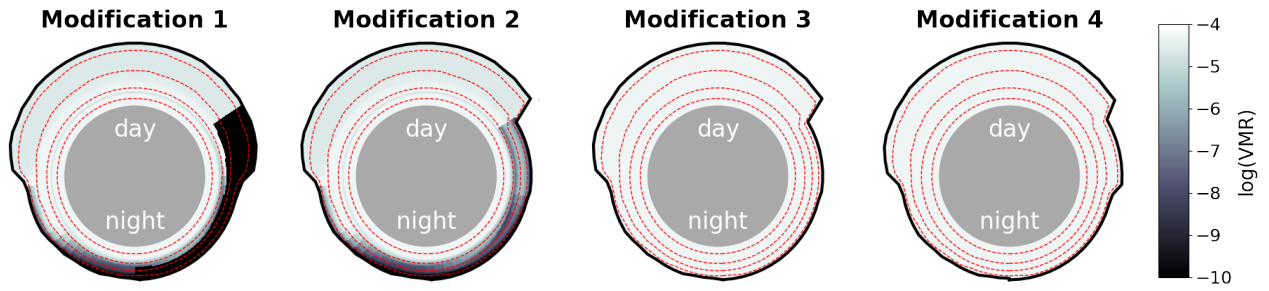


Figure 4.14: Iron abundances in the equatorial plane of the modified weak-drag models discussed in Section 4.5.3. In modification 1, all gaseous iron was removed from cells with longitudes $-180^\circ < \varphi < -58^\circ$ and pressures $P < 0.01$ bar. In modifications 2 and 3, the nightside temperature structure was extended up to -58° longitude, resulting in a smaller scale height on the leading limb. In modification 4, the leading limb has a constant temperature of 1800 K.

dances throughout the entire atmosphere, again with $\log(\text{VMR}) = -4.3$ for iron. As in the third row, we only consider Doppler shifts due to rotation when simulating the transit spectra. The uniform-temperature model does not exhibit any longitudinal variations and so the CCF peak heights of the individual sectors remain constant during the transit. In conjunction with the other plots in Fig. 4.11, this result proves that the observed changes in the signal strengths of the sectors are due to the 3D temperature structure of the atmosphere. Because the signal strengths of the uniform-temperature model remain constant, the global maximum in the CCF map of the full limb does not make a jump around mid-transit.

4.5.3 Nightside condensation of iron in the atmosphere of WASP-76b?

The match between our nominal model from Fig. 4.11 and the observations by Ehrenreich et al. (2020) and Kesseli & Snellen (2021) is not perfect yet. In the first half of the transit, the *observed* iron signals (see Fig. 4.1) blueshift a lot faster than the signal that results from our weak-drag atmosphere. As suggested by Ehrenreich et al. (2020), this discrepancy could be due to the fact that iron is in reality absent on the leading limb of WASP-76b. In what follows, our goal is (i) to check whether removing iron from the leading limb indeed results in a better match between the model and the data, and (ii) to explore whether the signal can be reproduced in any alternative way. To this end, we again apply a number of ad hoc modifications to the weak-drag model, which are summarised in Fig. 4.14.

To test the hypothesis from Ehrenreich et al. (2020), we take the nominal model from Fig. 4.11 and we remove gaseous iron from all atmospheric cells with longitudes⁷ $-180^\circ < \varphi < -58^\circ$ and pressures $P < 0.01$ bar. The resulting CCF maps are shown in the second row of Fig. 4.15 (modification 1). Modulo a small offset, the CCF map of the full limb provides a very good qualitative fit to the *observed* iron signal. Both RV curves exhibit a steep slope in the first half of the observation, followed by a clear “kink” around mid-transit, after which the net RV shift remains virtually constant.

The CCF maps of the individual limb sectors demonstrate how such an iron signal comes about. With respect to the nominal model, displayed in the top row, the maps of the trailing equator and the trailing pole are unaffected by the removal of iron. However, in the sectors on the leading limb, the iron signal fades away during the transit, as a larger part of the

⁷An upper limit $\varphi = -58^\circ$ was found to give the best match to the data after some trial and error.

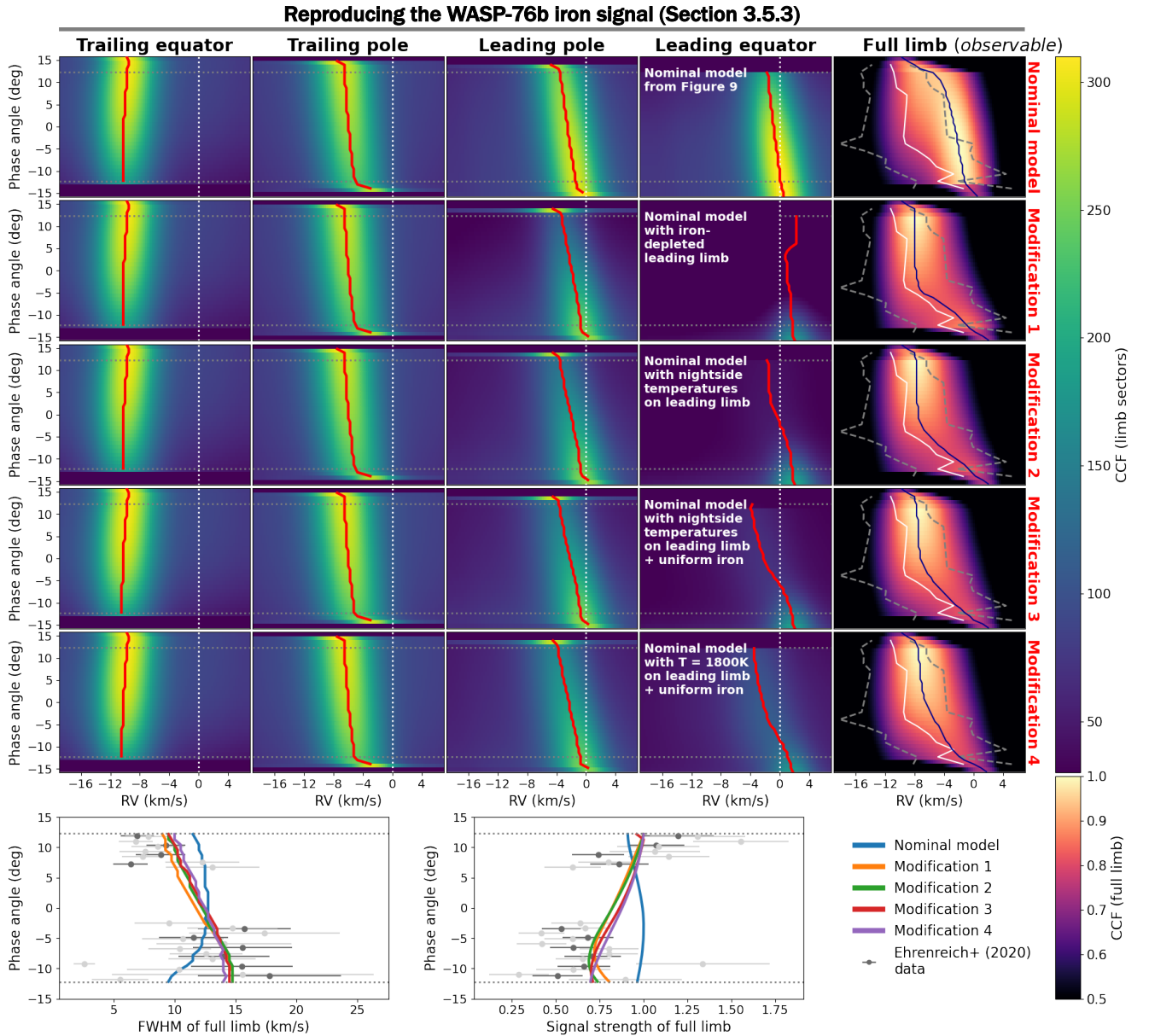


Figure 4.15: Same as Fig. 4.11, but now the nominal model was changed in such a way that the CCF map of the full limb resembles the WASP-76b signal as observed by [Ehrenreich et al. \(2020\)](#). In the panels in the right column, the white curve shows the peak position of the CCF that was obtained from VLT/ESPRESSO data, while the grey dashed lines indicate the corresponding FWHM. In the bottom panels, the FWHM and the signal strength of the models are plotted, along with data points from [Ehrenreich et al. \(2020\)](#).

dayside rotates out of view. In fact, on the leading equator, the CCF peak has completely disappeared in the second half of the observation. As far as the CCF map of the full limb is concerned, this means that the trailing limb starts to dominate the average over time, such that the signal is pulled towards more negative RVs in the second half of the transit.

In the third row of Fig. 4.15 (modification 2), we do not literally remove iron from the leading limb. Instead, we give all cells up to -58° longitude nightside temperatures, densities and abundances. As shown in Fig. 4.14, this also results in a scale-height asymmetry between the trailing and the leading limb of the atmosphere. The motivation for this heuristic model are the results from the previous sections, which show that the temperature structure can impact the signal strength of individual limb sectors over time (see Fig. 4.11). This has a direct effect on the cross-correlation signal of the full limb. It turns out that the CCF maps resulting from nightside temperatures on the leading limb are nearly identical to those of the nominal model with iron removed.

In the fourth row of Fig. 4.15 (modification 3), we take same model, but we additionally set the iron abundance to $\log(\text{VMR}) = -4.3$ across the *entire* atmosphere (see the structure in Fig. 4.14). In cells with $T < 1800$ K, we use the iron opacities at 1800 K, because iron would normally condense below this temperature. Remarkably, the CCF map of the full limb still provides an acceptable fit to the [Ehrenreich et al. \(2020\)](#) data, although the sharp kink around mid-transit has become less pronounced. This finding suggests that a substantial temperature difference between the planet's trailing and leading limb might be enough to reproduce the RV signal of WASP-76b – regardless of whether iron condensation occurs. Of course, it is very likely that iron clouds form on the leading limb when its temperature lies in the nightside regime. However, our simulations demonstrate that there could be (at least in theory) scenarios in which iron condensation is not strictly required to explain the planet's cross-correlation signal.

In the fifth row of Fig. 4.15 (modification 4), we take our approach one step further. Instead of setting the temperatures on the leading limb equal to those on the nightside, we assume a constant temperature of 1800 K, such that gaseous iron could in reality persist in this region. As shown in the right panel in Fig. 4.14, this also means that the leading limb is getting a larger scale height compared to the previous two models, such that its contribution to the total CCF will increase. As a result of these changes, the RV signal of the full limb loses its kink and the fit to the [Ehrenreich et al. \(2020\)](#) data becomes qualitatively worse. That said, the model still provides an insightful demonstration of the effect of temperature on the signal strength. Even though the trailing and leading equator have the same iron abundances, the signal of the latter remains much weaker because of its lower temperature.

The bottom-left panel in Fig. 4.15 shows the FWHM of the CCF maps of the full limb for the different modifications, as well as the nominal weak-drag model. The measurements from [Ehrenreich et al. \(2020\)](#) are plotted in the background. The data points come in two shades of grey, corresponding to different transit observations. Whereas the nominal model fails to match the data, the FWHM of the modified CCF maps seems to agree much better with the observations. In particular, the modified models correctly capture the *decrease* in the FWHM over time, from ~ 15 km/s at ingress to ~ 10 km/s at egress. In terms of signal strength (bottom-right panel in Fig. 4.15), the modified models also outperform the nominal weak-drag model. Their signal strength after ingress is $\sim 75\%$ of their signal strength before egress. This trend roughly matches the data, although the observations seem to suggest an even bigger change over time.

of the leading equator has a steeper slope and is more redshifted. Also, its lower peak values are likely due to Doppler broadening, caused by a larger variance of the line-of-sight velocities within the sector (see Fig. 4.9). As a result of these changes, the RV signal of the full limb has a somewhat steeper slope compared to the weak-drag model. Nonetheless, it is questionable to what degree observations can really differentiate between both atmospheres – that is, between a jet and a no-jet scenario.

The third row of Fig. 4.16 shows the CCF maps of the GCM model with strong drag ($\tau_{\text{drag}} = 10^4$ s). The shorter the drag timescale of the atmosphere, the further winds are slowed down. This effect is clearly visible on the trailing and leading equator, where the RV signals appear more redshifted compared to the weak-drag model. Reminiscent of the atmosphere in which the winds were set to zero (third row in Fig. 4.11), the CCF map of the full limb again features two modes. In the second half of the transit, the global maximum jumps from the marginally redshifted to the blueshifted mode.

The fourth row of Fig. 4.16 shows what happens to the CCF maps of the drag-free atmosphere when the opacities of TiO and VO are set to zero, both in the GCM and in HIRES-MCRT. As discussed in Section 4.3.1, this alters the radiation feedbacks in the GCM, and thereby the atmosphere’s temperature structure and wind profile (see Figs. 4.4–4.9). The CCF maps illustrate that the day-to-night winds in the drag-free atmosphere become stronger upon the removal of TiO and VO, because the RV signals shift to the left in every sector. Also, it is striking to see that the signals of the polar sectors and the leading equator become a lot weaker compared to the other models. Consequently, the strongly blueshifted signal of the trailing equator dominates in the second half of the observation, such that the global maximum in the CCF map of the full limb jumps to -12 km/s around mid-transit. Considering all four GCM atmospheres, the model without TiO and VO provides the best fit to the iron signal of WASP-76b (ignoring the modified atmospheres presented in Section 4.5.3). Although it does not manage to reproduce the kink in the RV signal, it does seem to give rise to the correct amount of blueshift. In the other GCM models, the blueshift is clearly too small, because the signal from the leading sectors does not fade quickly enough. Nonetheless, it remains an open question to what extent the absence of TiO and VO is a “competitive” explanation for the iron signal of WASP-76b. Recently, [Edwards et al. \(2020\)](#) claimed evidence for significant abundances of TiO and VO in the planet’s atmosphere, based on low-resolution emission spectra obtained with Hubble/WFC3. On the other hand, transmission spectra taken with the same instrument did not show a clear sign of either species.

With regards to Fig. 4.16 as a whole, it is important to note that the RV signals of the individual limb sectors show a number of general trends across the four atmospheric models – even though the CCF maps of the full limb may exhibit big differences. Firstly, all signals can be described by a straight line with a particular slope and offset. Also, the slopes have the same sign in each of the atmospheric scenarios. Furthermore, the signal strength of the trailing sectors always increases during the transit, while the strength of the leading sectors decreases over time. The rate of change is biggest in the equatorial regions, where cells move into (and out of) view the quickest. In other words, there is a correlation between a sector’s rotational velocity and the change observed in the local temperature structure.

In the light of these general trends, it may be possible to parametrise the sector signals, and to retrieve them from the CCF map of the *full limb* using an inverse-modelling technique. Although the feasibility of this method needs to be investigated, it could offer a unique way to extract spatial information from a planet’s CCF map. Of course, success will also depend

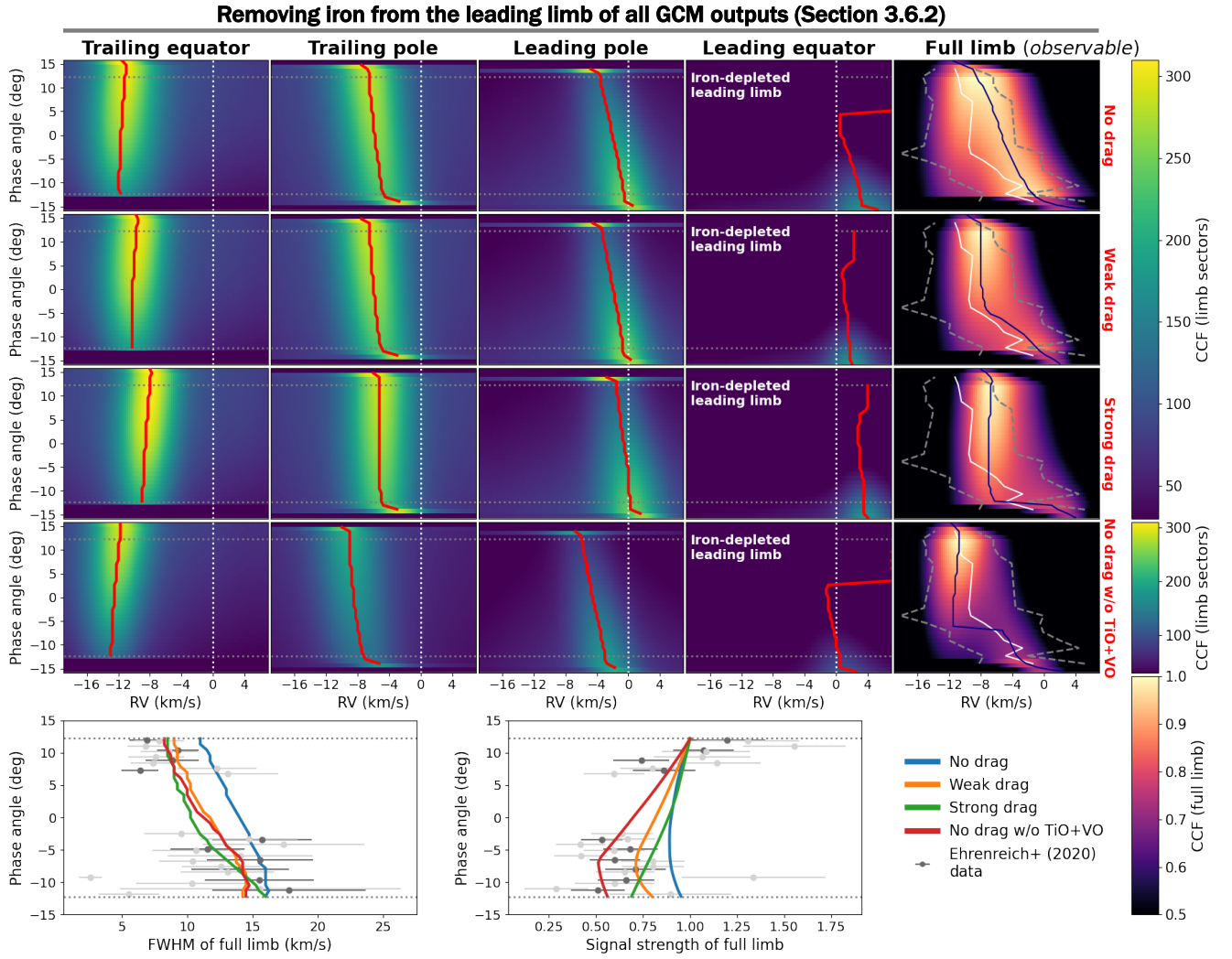


Figure 4.17: Same as Figs. 4.11, 4.15 and 4.16, but now for the four different GCM models with iron *removed* from the leading limb. All maps account for Doppler shifts due to atmospheric dynamics and planetary rotation.

on the quality of the data (compare both panels in Fig. 4.1), but with a new generation telescopes and high-resolution instruments coming up (e.g. VLT/CRIRES+ and E-ELT/HIRES), future observations have the power to reveal unprecedented amounts of information.

4.6.2 Removing iron from the leading limb

By analogy with the approach in Section 4.5.3, we now remove iron from the leading limb of the GCM atmospheres from Fig. 4.16 (again up to $\varphi = -58^\circ$) to investigate how the structure of their RV signal changes. The results are presented in Fig. 4.17, where the second row pertains to the weak-drag model discussed previously.

The first row of Fig. 4.17 shows the CCF maps of the drag-free model with iron removed from the leading limb. As far as the cross-correlations of the individual sectors are concerned, they appear very similar to those of the weak-drag model. However, the RV signals associated with the full limb show a clear discrepancy. Whereas the signal of the weak-drag model features a kink that is characteristic for the Ehrenreich et al. (2020) data, the RV slope

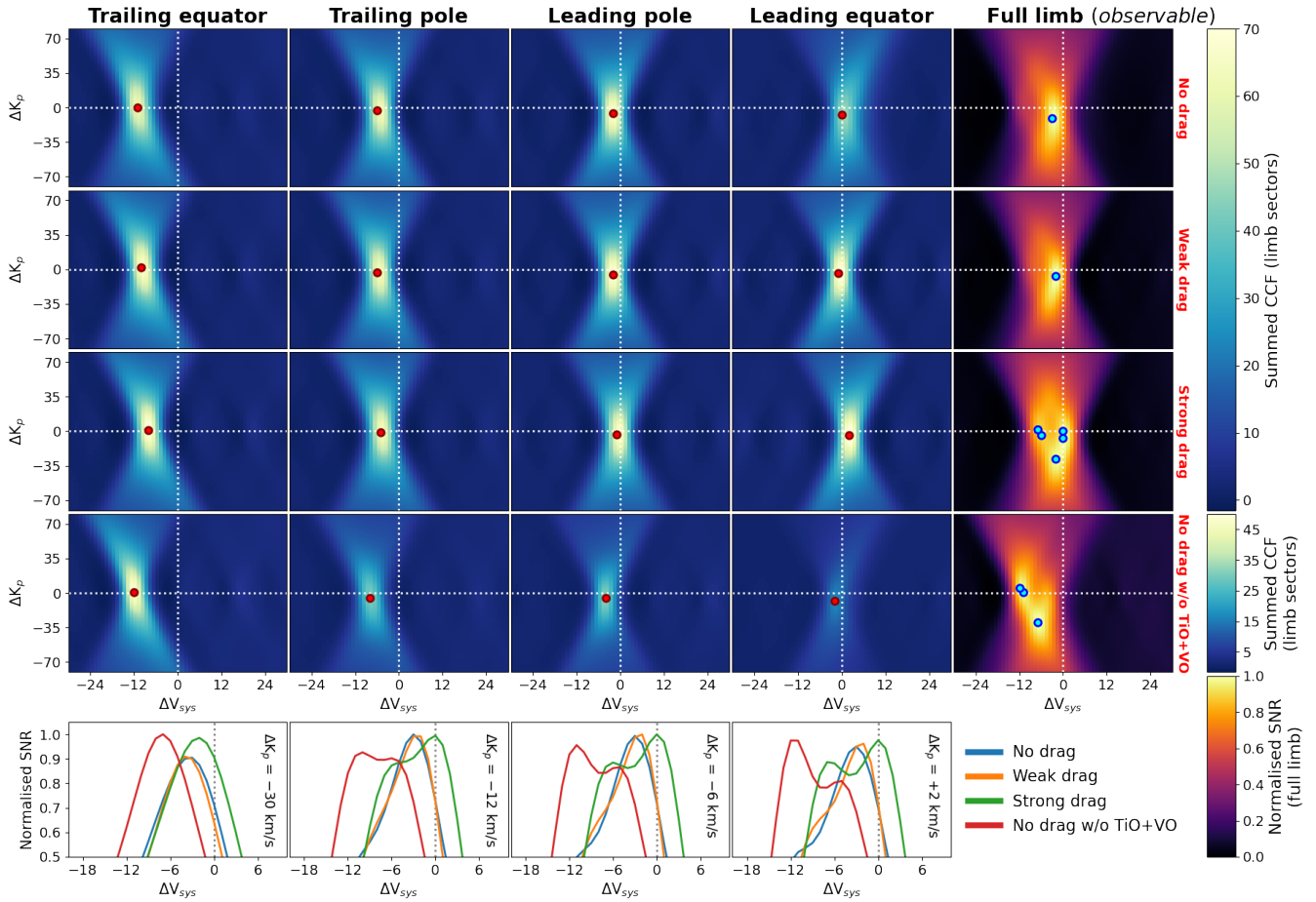


Figure 4.18: **Top four rows:** K_p - V_{sys} maps associated with the four GCM models from Fig. 4.16. In the panels pertaining to the limb sectors, we only summed (co-added) the CCF along the phase-axis, to provide a clear impression of a sector's contribution to the K_p - V_{sys} map of the full limb. The SNR values of the full limb were normalised between 0 and 1 to allow for an easy comparison between the different models. The bullet markers in each of the panels indicate local maxima. **Bottom panels:** Cross-sections of the K_p - V_{sys} maps of the full limb at four different values for ΔK_p .

of the drag-free model is more or less constant. A likely explanation for this is that the trailing equator of the drag-free model has a weaker signal compared to the weak-drag model, such that the impact of the trailing limb on the total average is smaller.

The third row of Fig. 4.17 shows the CCF maps associated with the strong-drag atmosphere. In comparison to the weak-drag model, the CCF map of the full limb provides a worse qualitative fit to the observed WASP-76b iron signal. The RV signal acquires an L-shape, because the signals of the trailing sectors lie relatively close together. As a result, they start to dominate the full-limb average early on, especially while the signals from the leading sectors are fading away.

The fourth row of Fig. 4.17 shows the CCF maps of the drag-free model without TiO and VO opacities. The signal of the trailing limb is stronger than that of the other sectors and because the leading limb is depleted of iron, the RV signal of the full limb jumps to -12 km/s after a third of the transit. In terms of overall blueshift, the CCF map provides a good fit to the observed WASP-76b iron signal. However, in terms of the *shape* of the RV signal, the fit is worse, because it features a jump rather than a kink.

4.7 K_p - V_{sys} maps of all GCM atmospheres

4.7.1 Nominal models

Fig. 4.18 shows the K_p - V_{sys} maps obtained for the four GCM models, whose CCF maps are displayed in Fig. 4.16. In this case, we only used the spectra from wavelength window 1 in Fig. 4.3, but we verified that the K_p - V_{sys} maps associated with window 2 are similar. Because we performed all simulations in the planetary rest frame, one would naively expect the SNR to peak at $(\Delta V_{\text{sys}}, \Delta K_p) = (0, 0)$ km/s. However, as the planet spectra are Doppler-shifted by winds and rotation, they may actually emulate the signal from a planet with a static atmosphere, but a nonzero system velocity and velocity semi-amplitude. As a consequence, the corresponding SNR maximum is displaced from $(0, 0)$ km/s. In general, the value of ΔV_{sys} is set by the *offset* of the RV signal in the cross-correlation map, while its *slope* determines the value of ΔK_p .

The first four columns of Fig. 4.18 show the K_p - V_{sys} maps associated with the individual limb sectors. The SNR was computed from equation 2.44, with $a = 1$ and $b = 0$, to allow for a comparison between the contributions from each of the sectors. The panels in the right column display the K_p - V_{sys} maps of the full limb, with a and b chosen such that the SNR ranges from zero to unity in each map. Fig. 4.18 illustrates that all limb sectors have a single SNR maximum, regardless of the atmospheric scenario. This is because one can fit a straight line with a well-defined slope and offset to the RV signals of the limb sectors in Fig. 4.16. In accordance with the CCF maps, the SNR maxima of the trailing equator are most blueshifted (most negative ΔV_{sys}), while the SNR maxima of the leading sectors are situated near $\Delta V_{\text{sys}} = 0$ km/s. Because the RV signals of the limb sectors only shift a couple of km/s during the transit, all SNR maxima lie close to $\Delta K_p = 0$ km/s.

The K_p - V_{sys} maps of the full limb are not necessarily single-peaked. Whereas the RV signals of the drag-free and the weak-drag model can be matched by a straight line (Fig. 4.16), the strong-drag model and the drag-free model without TiO and VO yield CCF maps with a more complicated structure. Their RV signals do not have a unique slope and offset, which leads to multiple maxima in K_p - V_{sys} space. Remarkably, this kind of behaviour was recently reported by Nugroho et al. (2020), who found a “double-peak” feature in the Fe I signal of MASCARA-2b/KELT-20b. After a thorough investigation into its origin, they suggested it may be a product of atmospheric dynamics. Also, Nugroho et al. (2020) were able to generate a K_p - V_{sys} map with multiple peaks from a fabricated CCF map that contained two separate trails – potentially analogous to separate contributions from a trailing and a leading limb.

Fig. 4.18 demonstrates that the locations of the SNR maxima of the full limb do not necessarily coincide with those of the individual limb sectors, as the sectors contribute only partially to the total signal. The map of the weak-drag model, for instance, looks diamond-shaped and features a local maximum at $(-2, -28)$ km/s. The K_p - V_{sys} map of the drag-free model without TiO and VO opacities acquires its highest value at $(-7, -30)$ km/s. These results show how relatively small RV shifts in a CCF map can lead to ΔK_p offsets of tens of km/s. When the RV signal features a jump, the best-fitting straight line automatically gets a steeper slope, associated with a large ΔK_p value.

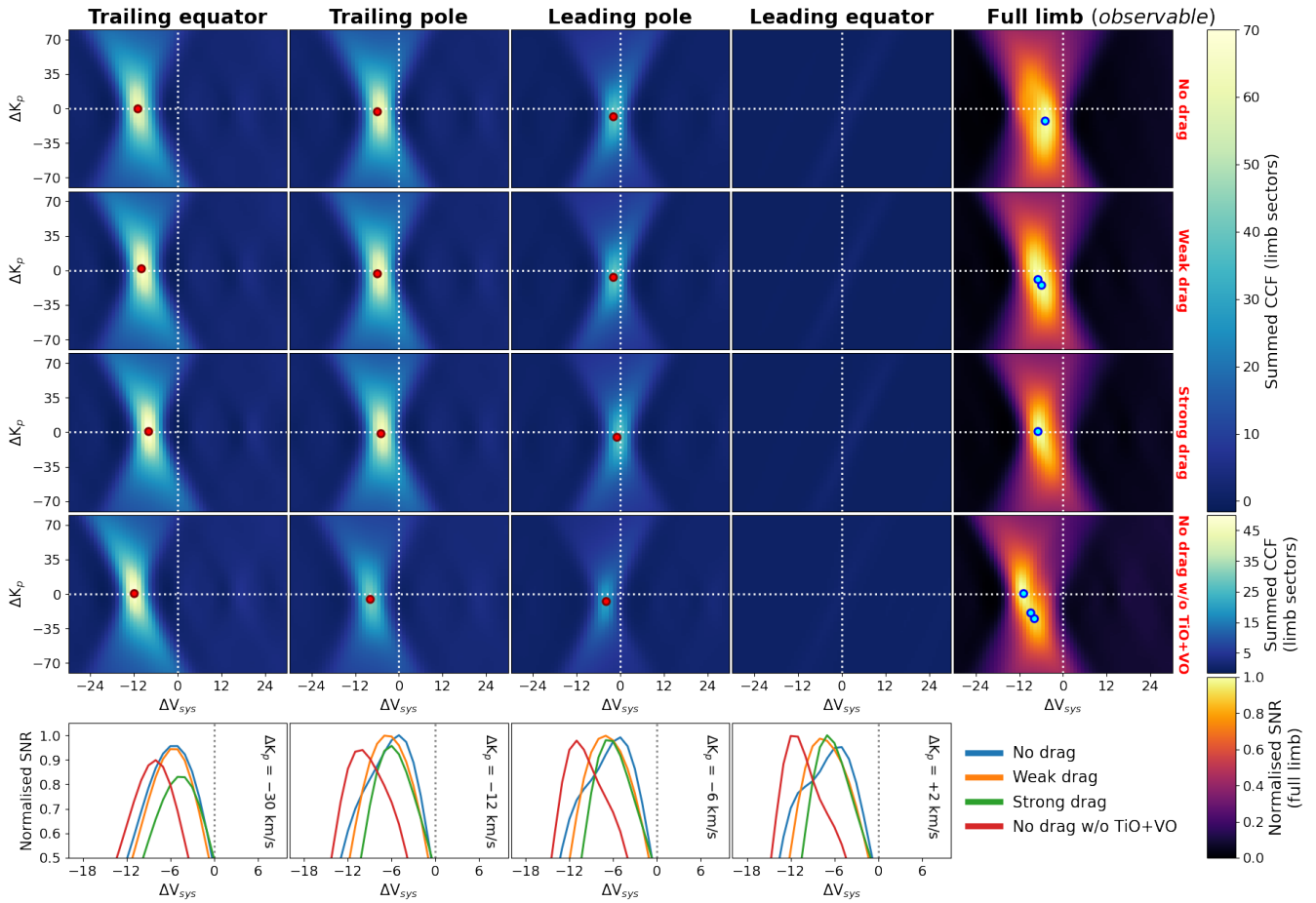


Figure 4.19: Same as Fig. 4.18, but now for the GCM models with iron removed from their leading limb. The corresponding CCF maps can be found in Fig. 4.17.

4.7.2 Removing iron from the leading limb

Fig. 4.19 shows what happens to the K_p - V_{sys} maps when iron is removed from the leading limb of the GCM atmospheres, just like in Sections 4.5.3 (modification 1) and 4.6.2. Because the contributions from the leading pole and leading equator fade, the SNR landscape is dominated by the trailing sectors. For the drag-free and the weak-drag model, this means that the SNR maxima of the full limb show further blueshift, away from (0,0) km/s. Moreover, the signal of the strong-drag model loses its diamond shape, because the redshift contribution from the leading equator is now zero. In this respect, a diamond-shaped K_p - V_{sys} map could indicate a *lack* of asymmetry between the trailing and the leading limb of a planet, although this needs to be verified more thoroughly. The maxima of the drag-free model without TiO and VO opacities appear less affected by the removal of iron from the atmosphere. This is because even without iron depletion, the signal from the trailing equator is already a lot stronger than that of the leading equator.

4.8 Studies published after 2021

In a similar spirit to this chapter, [Savel et al. \(2022\)](#) also post-processed GCM outputs to assess the effect of limb-asymmetries on the iron signal of WASP-76b. Rather than modifying the GCM output (as we did in Fig. 4.14), they only removed iron from regions where the temperature structure allowed for it (i.e., all regions of the atmosphere cooler than the condensation temperature of iron). They found that their model produced an increasing blueshift over time. However, it could not match the -10 km/s blueshift observed with ESPRESSO in the second half of the transit. To try and further reduce the contribution from the leading limb, [Savel et al. \(2022\)](#) added optically thick clouds composed of Al_2O_3 , Fe, and Mg_2SiO_4 to the atmosphere, again in a way consistent with the 3D temperature structure (see also Chapter 6). This enhanced the blueshift in the second half of the transit by ~ 0.5 km/s. Finally, they reported that a better fit to the data could be obtained when allowing the orbit of WASP-76b to be slightly eccentric ($e \approx 0.017$). Although this result is consistent with current constraints on the planet’s orbit ([West et al. 2016](#), [Fu et al. 2021](#)), it is uncertain whether a nonzero eccentricity fits into the dynamical picture of UHJs (e.g., [Rasio et al. 1996](#)). Also, an asymmetric iron signal has been observed in the atmosphere of WASP-121b ([Borsa et al. 2021](#)), for which the eccentricity is more tightly constrained ([Bourrier et al. 2020b](#)).

[Gandhi et al. \(2022, incl. Wardenier\)](#) performed a (pseudo-)2D retrieval on the ESPRESSO data from [Ehrenreich et al. \(2020\)](#), employing a combination of two 1D forward models to separately account for the trailing and leading limbs of the planet. They also performed separate retrievals on the first and the last quarter of the transit (avoiding the Doppler shadow of the star during the central half), thus obtaining four sets of posteriors – two for each limb. [Gandhi et al. \(2022\)](#) reported tight constraints on the iron abundance on the trailing limb in the last quarter of the transit (see Fig. 4.20). They also retrieved day-to-night wind speeds of ~ 5.9 km/s in the first quarter and ~ 9.8 km/s in the last quarter. The iron abundance on the leading limb could be less well constrained due to a degeneracy with the altitude of the optically thick cloud deck included in the model. The latter is indicative of the fact that the spectrum contains less information about the leading limb of the planet. Overall, [Gandhi et al. \(2022\)](#) found that the 2D retrieval was statistically preferred by 4.9σ over a regular phase-combined 1D retrieval, highlighting the 3D nature of WASP-76b.

Fig. 4.21 shows a comparison between the best-fit spectra found by [Gandhi et al. \(2022\)](#) (one for each quarter) and the spectra of the cold-morning-limb model (see “modification 2” in Fig. 4.14) presented in this chapter. The spectra from [Gandhi et al. \(2022\)](#) were obtained by averaging the outputs of the 1D models associated with both limbs. In the first quarter of the transit (when the dayside is in view on the leading limb), there is excellent agreement between the 2D model and the (modified) GCM output. The absorption lines in the GCM spectrum, however, show more detailed features. This is because the GCM output has a 3D wind profile, while the forward models in the retrieval used a single wind kernel to shift and broaden the absorption lines. In the final quarter (where the dayside is in view on the trailing limb), the spectra still match well in terms of line position and line width. Yet, the retrieved best-fit spectrum has a smaller line contrast. [Gandhi et al. \(2022\)](#) suggested a few possible reasons for this. Firstly, the retrieved spectrum is an actual fit to the ESPRESSO data, while the GCM output is not. Secondly, the retrieved temperature of the dayside on the trailing limb is ~ 3000 K, while the dayside temperatures of the GCM reach 3500 K. Locally, this results in larger scale heights and stronger iron opacities in the GCM, increasing the line strength of the [Wardenier et al. \(2021\)](#) spectrum in Fig. 4.21.

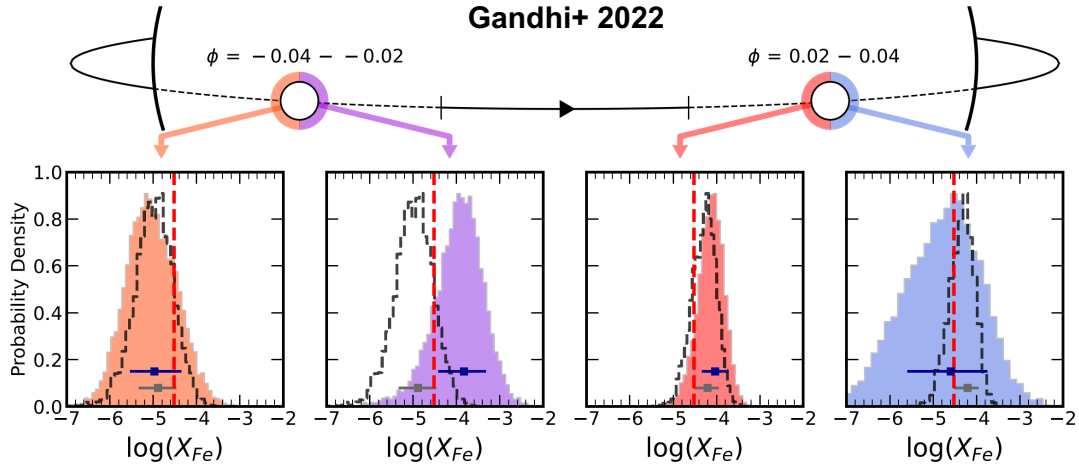


Figure 4.20: Results from the 2D retrieval by Gandhi et al. (2022), performed on transit data of WASP-76b. The study retrieved the atmospheric properties on the trailing limb (orange and red) and the leading limb (purple and blue) of the planet, during the first quarter $\phi \in [-0.04, -0.02]$ and the final quarter $\phi \in [0.02, 0.04]$ of the transit. The coloured histograms show the iron abundance retrieved for each part of the atmosphere (with the *blue bar* indicating the median and the 1σ uncertainty). The dashed histograms show the result of a 1D retrieval, applied to the first quarter and the final quarter of the transit, respectively (with the *grey bar* indicating the median and the 1σ uncertainty). Red dashed lines indicate the solar iron abundance. Figure courtesy of Gandhi et al. (2022).

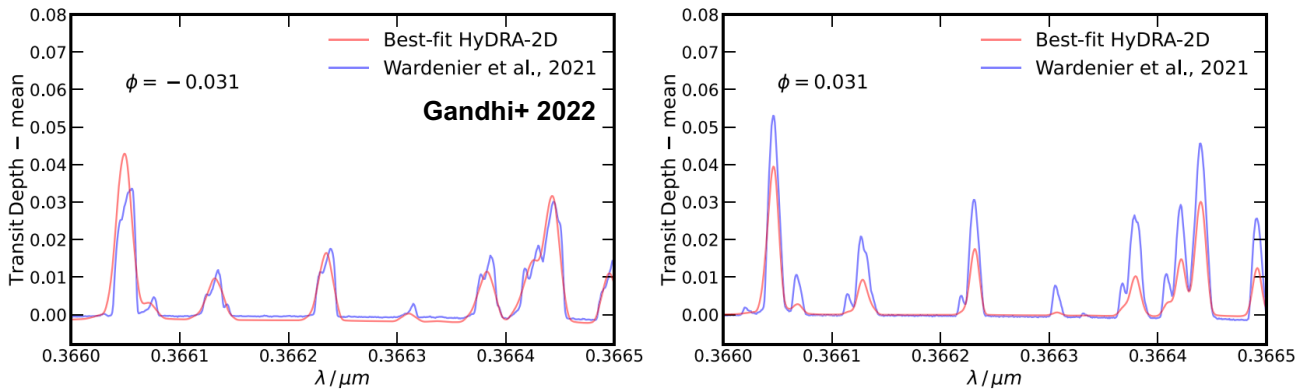


Figure 4.21: Best-fit spectra from the 2D retrieval performed by Gandhi et al. (2022). The left panel shows the best-fit spectrum (in red) for the *first* quarter of the transit and the right panel shows the best-fit spectrum (in red) for the *final* quarter of the transit. Spectra of the best-fitting model found in this chapter (Wardenier et al. 2021) are shown in blue. Figure courtesy of Gandhi et al. (2022).

4.9 Summary & conclusion

Interpreting spectra that originate from inherently 3D exoplanet atmospheres is a challenge. This is especially true for ultra-hot Jupiters, which are characterised by an extreme day-night temperature contrast that drives a complex atmospheric circulation pattern. Because transmission spectroscopy probes the terminator of the atmosphere, it is sensitive to the regions where the largest thermal and chemical gradients occur. Since the transit of an ultra-hot Jupiter typically subtends a large angle ($\sim 30^\circ$ in the case of WASP-76b), the high-resolution spectrum of the planet can undergo significant changes with time (see Fig. 4.10), and this complicates the cross-correlation signal in the planetary rest frame. Many observational

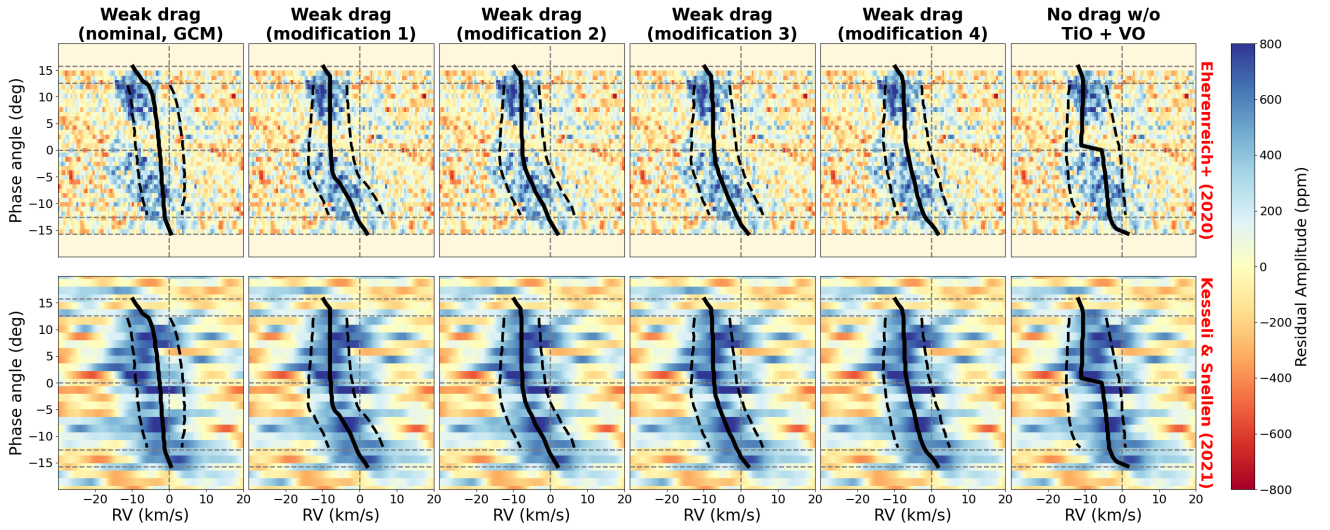


Figure 4.22: The CCF maps from Ehrenreich et al. (2020) (top row) and Kesseli & Snellen (2021) (bottom row), with some of the models presented in this chapter plotted on top. The left column shows the nominal weak-drag model from the GCM (discussed in Section 4.5.1), while the four central columns show the modified weak-drag models covered in Section 4.5.3. As shown in Fig. 4.14, Modification 1 has an iron-depleted leading limb, modification 2 has nightside temperatures on the leading limb, modification 3 has nightside temperatures on the leading limb and uniform iron abundances, while modification 4 has a leading limb of 1800 K and uniform iron abundances. The right column depicts the signal obtained from the drag-free atmosphere without TiO and VO opacities (see Section 4.6.1). This is the GCM model that comes closest to the data without making any changes to the atmospheric structure.

studies have reported Doppler shifts in the absorption signals of ultra-hot Jupiters, but a clear picture of the dependencies is still lacking. This is why we require 3D frameworks to draw concrete links between (i) an atmosphere’s structure, composition and dynamics, and (ii) the observed spectra.

In this chapter, we used the SPARC/MITgcm to simulate different atmospheric scenarios of the ultra-hot Jupiter WASP-76b (see Section 4.3.1). We considered models with three different drag timescales. Also, we investigated the effect of setting TiO and VO opacities to zero in the drag-free model. We then employed a Monte-Carlo radiative transfer code, HIRES-MCRT (the predecessor of gCMCRT), to compute high-resolution transmission spectra with iron (Fe I) lines at 37 orbital phases during the transit. HIRES-MCRT randomly draws transit chords along the line of sight, for which the optical depth is computed in a 3D spherical geometry. The transmission spectrum is then found by averaging over a sufficiently large sample of photon packets (see equation 2.8).

The (phase-dependent) signal from the full limb of the planet can be hard to interpret due to the interplay between temperature, chemistry, dynamics and rotation. Hence, we decomposed the atmospheric annulus into four limb sectors (see Fig. 2.2) and analysed the cross-correlation signals from each of the sectors separately. In the end, the cross-correlation map of the full limb is equal to the average of the maps of the individual sectors (see equation 2.41).

By applying simple modifications to the weak-drag model (see Fig. 4.11), we were able to identify the impact of the iron distribution and the temperature structure on the cross-correlation signal. We showed that the introduction of uniform iron abundances hardly

alters the final observable. On the other hand, the vast temperature difference between the dayside and nightside causes the signal strengths of the sectors to change over time, and this affects the structure of the cross-correlation map. In addition, we investigated the nature of the WASP-76b iron signal observed by [Ehrenreich et al. \(2020\)](#) and [Kesseli & Snellen \(2021\)](#). We demonstrated that the signal can be qualitatively reproduced by (i) removing gaseous iron from the leading limb of the weak-drag model and not changing the temperature structure, or (ii) applying a large temperature difference between the trailing and the leading limb of the planet. In case (ii), one might argue that a model without iron condensation provides a sufficiently good match to the data (see Figs. 4.14 and 4.15), although iron condensation becomes inevitable when the temperature (and thereby the scale height) on the leading limb is further reduced. That said, the kink in the signal is most pronounced when iron is completely gone. Since our work was mainly exploratory, follow-up studies will have to shed light on the physical mechanisms that can give rise to (apparently large) asymmetries between the trailing and the leading limb of ultra-hot Jupiters.

In Section 4.6.1, we computed the cross-correlation maps of all four GCM atmospheres (see Figs. 4.16 and 4.17), and we showed that the drag timescale can have a substantial impact on the structure of the cross-correlation map. This is because the planet’s wind profile governs the slopes and offsets of the RV signals originating from the limb sectors. We also showed that the cross-correlation map of the drag-free atmosphere changes drastically upon the removal of TiO and VO opacities, mainly because the new temperature structure affects the relative strength of the signals associated with individual sectors. Finally, the K_p – V_{sys} maps of the GCM atmospheres were presented in Section 4.7, and we showed that atmospheric dynamics can give rise to multiple SNR maxima that are displaced from (0,0) km/s in the planetary rest frame.

Our most important conclusions are summarised below:

- The cross-correlation map of an ultra-hot Jupiter primarily encodes information about its temperature structure, dynamics and rotation. Based on the cross-correlation map, it is not possible to differentiate between (i) an atmosphere with uniform iron abundances and (ii) an atmosphere with equilibrium chemistry, where iron condenses at low (nightside) temperatures (see Figs. 4.11 and 4.15). Of course, this holds as long as the abundances on the trailing and the leading limb are high enough to be detected.
- The temperature contrast between the dayside and the nightside causes the signal strengths associated with limb sectors to change during the transit (see Fig. 4.11). The hotter a region probed by the observation, the stronger the iron signal becomes (see Fig. 4.13). Changes are biggest around the equator, where atmospheric regions move into (or out of) view the quickest. Due to these variations, the RV signal of an ultra-hot Jupiter may feature jumps or kinks (see e.g., Figs. 4.16 and 4.17).
- Atmospheric drag can have a considerable impact on the cross-correlation signal of ultra-hot Jupiters, because it slows down winds and suppresses jet formation. In the regime of strong drag ($\tau_{\text{drag}} \sim 10^4$ s), the cross-correlation signal features two modes (see Fig. 4.16) that cause the global maximum to jump from 0 to -6 km/s after mid-transit.
- Removing TiO and VO opacities from the drag-free model drastically alters the tem-

perature structure of the atmosphere. The hotspot shift on the dayside extends to higher altitudes, such that the temperature (and scale-height) asymmetry between the trailing and leading limb is larger than in the other models (see Fig. 4.4). This causes the signal of the hotter, blueshifted trailing equator to be much stronger than the signals of the other limb sectors.

- The iron signal of WASP-76b reported by [Ehrenreich et al. \(2020\)](#) and [Kesseli & Snellen \(2021\)](#) can be reproduced by removing iron from the leading limb of the weak-drag model, up to a longitude of $\phi \approx -58^\circ$. Additionally, the signal can be reasonably well matched by models with uniform iron abundances and a large temperature difference between the trailing and the leading limb (see Figs. 4.14 and 4.15). In these scenarios, iron condensation (although likely to happen) is not strictly required.
- When iron is removed from the leading limb, the weak-drag model ($\tau_{\text{drag}} \sim 10^5$ s) provides a better fit to the WASP-76b observations than the other GCM atmospheres (see Fig. 4.17). In fact, it is the only model that can reproduce the kink in the RV signal.
- Atmospheric dynamics and rotation can cause the peak in the K_p - V_{sys} map to be substantially displaced from (0,0) km/s in the planetary rest frame, especially along the K_p axis (see Figs. 4.18 and 4.19). Additionally, there can be multiple (local) SNR maxima when the RV signal of the planet deviates too much from a single straight line. The K_p - V_{sys} map of the strong-drag model, for instance, exhibits a diamond shape.

Bibliography

- Allard N. F., Allard F., Hauschildt P. H., Kielkopf J. F., Machin L., 2003, [A&A](#), 411, L473
- Allard N. F., Spiegelman F., Kielkopf J. F., 2016, [A&A](#), 589, A21
- Arcangeli J., et al., 2019, [A&A](#), 625, A136
- Beatty T. G., Madhusudhan N., Tsaras A., Zhao M., Gilliland R. L., Knutson H. A., Shporer A., Wright J. T., 2017, [AJ](#), 154, 158
- Beltz H., Rauscher E., Brogi M., Kempton E. M. R., 2021, [AJ](#), 161, 1
- Bernath P. F., 2020, [J. Quant. Spectrosc. Radiative Transfer](#), 240, 106687
- Blecic J., Dobbs-Dixon I., Greene T., 2017, [ApJ](#), 848, 127
- Borsa F., et al., 2021, [A&A](#), 645, A24
- Bourrier V., et al., 2020a, [A&A](#), 635, A205
- Bourrier V., et al., 2020b, [A&A](#), 637, A36
- Caldas A., Leconte J., Selsis F., Waldmann I. P., Bordé P., Rocchetto M., Charnay B., 2019, [A&A](#), 623, A161
- Cauley P. W., Shkolnik E. L., Ilyin I., Strassmeier K. G., Redfield S., Jensen A., 2019, [AJ](#), 157, 69
- Edwards B., et al., 2020, [AJ](#), 160, 8
- Ehrenreich D., et al., 2020, [Nature](#), pp 1–7
- Feng Y. K., Line M. R., Fortney J. J., Stevenson K. B., Bean J., Kreidberg L., Parmentier V., 2016, [ApJ](#), 829, 52
- Flowers E., Brogi M., Rauscher E., Kempton E. M.-R., Chiavassa A., 2019, [AJ](#), 157, 209
- Fortney J., Lodders K., Marley M., Freedman R., 2008, [ApJ](#), 678, 1419
- Fortney J. J., Shabram M., Showman A. P., Lian Y., Freedman R. S., Marley M. S., Lewis N. K., 2010, [ApJ](#), 709, 1396
- Fu G., et al., 2021, [AJ](#), 162, 108
- Gandhi S., Madhusudhan N., 2019, [MNRAS](#), 485, 5817
- Gandhi S., Kesseli A., Snellen I., Brogi M., Wardenier J. P., Parmentier V., Welbanks L., Savel A. B., 2022, [MNRAS](#), 515, 749

- Gharib-Nezhad E., Iyer A. R., Line M. R., Freedman R. S., Marley M. S., Batalha N. E., 2021a, EXOPLINES: Molecular Absorption Cross-Section Database for Brown Dwarf and Giant Exoplanet Atmospheres, [doi:10.5281/zenodo.4458189](https://doi.org/10.5281/zenodo.4458189), <https://doi.org/10.5281/zenodo.4458189>
- Gharib-Nezhad E., Iyer A. R., Line M. R., Freedman R. S., Marley M. S., Batalha N. E., 2021b, *ApJS*, **254**, 34
- Harada C. K., Kempton E. M. R., Rauscher E., Roman M., Malsky I., Brinjikji M., DiTomaso V., 2021, *ApJ*, **909**, 85
- Hoeijmakers H. J., et al., 2019, *A&A*, **627**, A165
- Hoeijmakers H. J., et al., 2020, *A&A*, **641**, A120
- Hubeny I., Burrows A., Sudarsky D., 2003, *ApJ*, **594**, 1011
- John T. L., 1988, *A&A*, **193**, 189
- Kataria T., Showman A. P., Fortney J. J., Stevenson K. B., Line M. R., Kreidberg L., Bean J. L., Désert J.-M., 2015, *ApJ*, **801**, 86
- Kataria T., Sing D. K., Lewis N. K., Visscher C., Showman A. P., Fortney J. J., Marley M. S., 2016, *ApJ*, **821**, 9
- Keles E., 2021, *MNRAS*, **502**, 1456
- Kempton E. M.-R., Perna R., Heng K., 2014, *ApJ*, **795**, 24
- Kesseli A. Y., Snellen I. A. G., 2021, *ApJ*, **908**, L17
- Komacek T. D., Showman A. P., 2016, *ApJ*, **821**, 16
- Komacek T. D., Showman A. P., Tan X., 2017, *ApJ*, **835**
- Kurucz R., Bell B., 1995, Atomic Line Data (R.L. Kurucz and B. Bell) Kurucz CD-ROM No. 23. Cambridge, **23**
- Lacy B. I., Burrows A., 2020, *ApJ*, **905**, 131
- Lewis N. K., Parmentier V., Kataria T., de Wit J., Showman A. P., Fortney J. J., Marley M. S., 2017, arXiv e-prints, p. [arXiv:1706.00466](https://arxiv.org/abs/1706.00466)
- Li J., Goodman J., 2010, *ApJ*, **725**, 1146
- Line M. R., Parmentier V., 2016, *ApJ*, **820**, 78
- MacDonald R. J., Madhusudhan N., 2017, *MNRAS*, **469**, 1979
- MacDonald R. J., Goyal J. M., Lewis N. K., 2020, *ApJ*, **893**, L43
- Mendonça J. M., Tsai S.-m., Malik M., Grimm S. L., Heng K., 2018, *ApJ*, **869**, 107
- Miller-Ricci Kempton E., Rauscher E., 2012, *ApJ*, **751**, 117
- Nugroho S. K., Gibson N. P., de Mooij E. J. W., Watson C. A., Kawahara H., Merritt S., 2020, *MNRAS*, **496**, 504
- Nugroho S. K., et al., 2021, *ApJ*, **910**, L9
- Parmentier V., Crossfield I. J. M., 2018, Exoplanet Phase Curves: Observations and Theory. Springer, p. 116, [doi:10.1007/978-3-319-55333-7_116](https://doi.org/10.1007/978-3-319-55333-7_116)
- Parmentier V., Guillot T., 2014, *A&A*, **562**, A133
- Parmentier V., Showman A. P., Lian Y., 2013, *A&A*, **558**, 91
- Parmentier V., Fortney J. J., Showman A. P., Morley C., Marley M. S., 2016, *ApJ*, **828**, 22
- Parmentier V., et al., 2018, *A&A*, **617**
- Parmentier V., Showman A. P., Fortney J. J., 2021, *MNRAS*, **501**, 78
- Perna R., Menou K., Rauscher E., 2010a, *ApJ*, **719**, 1421
- Perna R., Menou K., Rauscher E., 2010b, *ApJ*, **724**, 313
- Pluriel W., Zingales T., Leconte J., Parmentier V., 2020, *A&A*, **636**, A66
- Rainer M., et al., 2021, *A&A*, **649**, A29
- Rasio F. A., Tout C. A., Lubow S. H., Livio M., 1996, *ApJ*, **470**, 1187
- Rauscher E., Kempton E. M. R., 2014, *ApJ*, **790**, 79
- Rauscher E., Menou K., 2012, *ApJ*, **750**, 96
- Savel A. B., et al., 2022, *ApJ*, **926**, 85
- Seidel J. V., Ehrenreich D., Pino L., Bourrier V., Lavie B., Allart R., Wyttenbach A., Lovis C., 2020, *A&A*, **633**, A86
- Showman A. P., Polvani L. M., 2011, *ApJ*, **738**, 71
- Showman A. P., Fortney J. J., Lian Y., Marley M. S., Freedman R. S., Knutson H. A., Charbonneau D., 2009, *ApJ*, **699**, 564
- Showman A. P., Fortney J. J., Lewis N. K., Shabram M., 2013, *ApJ*, **762**
- Showman A. P., Lewis N. K., Fortney J. J., 2015, *ApJ*, **801**, 95
- Spiegel D. S., Silverio K., Burrows A., 2009, *ApJ*, **699**, 1487
- Stangret M., Casasayas-Barris N., Pallé E., Yan F., Sánchez-López A., López-Puertas M., 2020, *A&A*, **638**, A26
- Steinrueck M. E., Parmentier V., Showman A. P., Lothringer J. D., Lupu R. E., 2019, *ApJ*, **880**, 14
- Steinrueck M. E., Showman A. P., Lavvas P., Koskinen T., Tan X., Zhang X., 2021, *MNRAS*, **504**, 2783

- Tan X., Komacek T. D., 2019, [ApJ](#), 886, 26
- Taylor J., Parmentier V., Irwin P. G. J., Aigrain S., Lee G. K. H., Krissansen-Totton J., 2020, [MNRAS](#), 493, 4342
- Tennyson J., et al., 2020, [J. Quant. Spectrosc. Radiative Transfer](#), 255, 107228
- Visscher C., Lodders K., Fegley B., 2010, [ApJ](#), 716, 1060
- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, [MNRAS](#), 506, 1258
- West R. G., et al., 2016, [A&A](#), 585, A126
- Zhang J., Kempton E. M.-R., Rauscher E., 2017, [ApJ](#), 851, 84

Chapter 5

All along the line of sight: A closer look at opening angles and absorption regions in the atmospheres of transiting exoplanets

The material in this chapter is based on [Wardenier et al. \(2022\)](#):

– Wardenier J. P., Parmentier V., Lee E. K. H., 2022, MNRAS, 510, 620

Abstract – *Transmission spectra contain a wealth of information about the atmospheres of transiting exoplanets. However, large thermal and chemical gradients along the line of sight can lead to biased inferences in atmospheric retrievals. In order to determine how far from the limb plane the atmosphere still impacts the transmission spectrum, we derive a new formula to estimate the opening angle of a planet. This is the angle subtended by the atmospheric region that contributes to the observation along the line of sight, as seen from the planet centre. We benchmark our formula with a 3D Monte-Carlo radiative transfer code and we define an opening angle suitable for the interpretation of JWST observations, assuming a 10-ppm noise floor. We find that the opening angle is only a few degrees for planets cooler than ca. 500 Kelvins, while it can be as large as 25 degrees for (ultra-)hot Jupiters and 50 degrees for hot Neptunes. Compared to previous works, our more robust approach leads to smaller estimates for the opening angle across a wide range scale heights and planetary radii. Finally, we show that ultra-hot Jupiters have an opening angle that is smaller than the angle over which the planet rotates during the transit. This allows for time-resolved transmission spectroscopy observations that probe independent parts of the planetary limb during the first and second half of the transit.*

5.1 Introduction

Over the past two decades, transmission spectroscopy (e.g., [Seager & Sasselov 2000](#); [Charbonneau et al. 2002](#); [Snellen et al. 2008](#); [Sing et al. 2016](#); [Nikolov et al. 2018](#)) has been integral to the atmospheric characterisation of transiting exoplanets – constraining their chemical abundances and temperature profiles. When an exoplanet passes in front of its host star, a small fraction of the stellar photons are absorbed and scattered by the planetary atmosphere. Because the atmosphere’s opacity is wavelength-dependent, measuring the effective radius of the planet $R_{\text{eff}}(\lambda)$ at different wavelengths results in a transmission spectrum. The transmission spectrum is generally expressed in terms of a depth $\delta(\lambda) = R_{\text{eff}}(\lambda)^2 / R_{\star}^2$, with $R_{\star}$ the radius of the host star.

In order to physically interpret a transmission spectrum and infer the properties of the underlying atmosphere, it is essential to know what regions of the atmosphere are actually probed by the observation. In 1D radiative-transfer models, it is possible to compute a so-called *transmission contribution function* (TCF, [Barstow et al. 2013](#); [Mollière et al. 2019](#)), which quantifies how substantially an atmospheric layer contributes to the spectrum at a given wavelength. The basic idea is to switch off (or perturb) the opacities layer-by-layer and compute the resulting transit radius of the planet. The greater the deviation from the original radius, the greater the contribution by the associated layer. In this way, the TCF can

be seen as the derivative of the transmission with respect to pressure.

Because exoplanet atmospheres are 3D, the atmospheric region probed by transmission spectroscopy – henceforth called the *absorption region* – does not only extend along the altitude axis, but also along the line of sight, perpendicular to the limb plane. 1D models that are typically used to interpret observations ignore this dimension (e.g., [Line et al. 2013](#); [Waldmann et al. 2015](#); [Mollière et al. 2019](#)). However, a collection of recent works ([Caldas et al. 2019](#); [Lacy & Burrows 2020](#); [Pluriel et al. 2020, 2021](#)) have shown that thermal and chemical gradients between the dayside and nightside of tidally locked gas giants can have a significant impact on their transmission spectrum – for earlier studies that computed spectra from 3D models, see [Burrows et al. \(2010\)](#) and [Fortney et al. \(2010\)](#). Therefore, it is valuable to assess *how far* from the limb plane the atmosphere still influences a planet’s transmission spectrum, and thus *how stretched* the absorption region is along the line of sight. Essentially, we require a TCF for the line-of-sight dimension.

The absorption region can be seen as a “resolution element”. If the absorption region is compact, the transmission spectrum probes a very specific part of the atmosphere, with its own temperature and chemistry. On the other hand, if the absorption region is stretched along the line of sight, the transmission spectrum is shaped by the atmospheric structure across many different longitudes. In the context of tidally locked planets, this has important implications. Ultra-hot Jupiters ([Arcangeli et al. 2018](#); [Bell & Cowan 2018](#); [Parmentier et al. 2018](#)), for example, rotate by tens of degrees during a transit, owing to their short orbital radii.¹ Hence, one can expect observations to probe different longitudes at different orbital phases (e.g., Chapter 4; [Bourrier et al. 2020](#); [Ehrenreich et al. 2020](#); [Hoeijmakers et al. 2020](#); [Borsa et al. 2021](#); [Kesseli & Snellen 2021](#)). However, it is the resolution element that determines how independent the measurements (of wind speeds, temperature and composition) at the various orbital phases are. The size of the absorption region governs how much local information can be retrieved from the transmission spectrum.

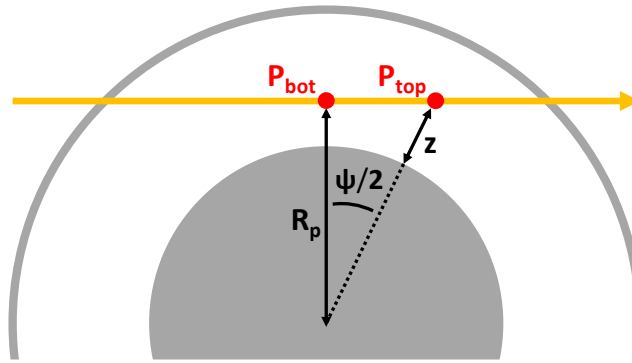
The goal of this chapter is to obtain an estimate for the extent of the absorption region along the line of sight – and thus assess the importance of accounting for this dimension when interpreting observations. In Section 5.2, we briefly discuss work that has already been done in this regard. In Section 5.3, we derive a new analytical formula for the opening angle (i.e. the angular extent of the absorption region along the line of sight) and we validate it using a Monte-Carlo radiative transfer code. In Section 5.4, we study the wavelength dependence of the absorption region and the opening angle. In Section 5.5, we assess how the opening angle behaves when an instrument noise floor is assumed. Finally, we discuss the implications of this work in Section 5.6, followed by a conclusion in Section 5.7.

5.2 Previous work

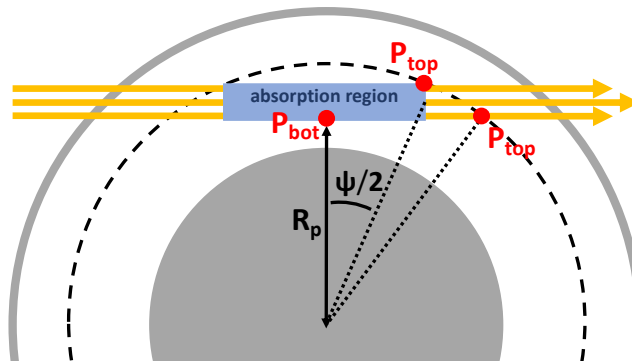
[Caldas et al. \(2019\)](#) used a geometrical argument to estimate what portion of the atmosphere is probed along the line of sight. To this end, they introduced the opening angle ψ . This is the angle (as seen from the centre of the planet) subtended by the region that contributes to the observation. The top panel of Fig. 5.1 illustrates how ψ can be computed. Firstly, one has to assume a minimum pressure P_{top} and a maximum pressure P_{bot} between which the

¹Under the assumption of tidal locking, WASP-76b and WASP-121b (two typical ultra-hot Jupiters) rotate by 31 and 35 degrees during their transit, respectively. This includes the ingress and egress phase.

(A) Single wavelength, single transit chord



(B) Single wavelength, multiple transit chords



(C) Multiple wavelengths

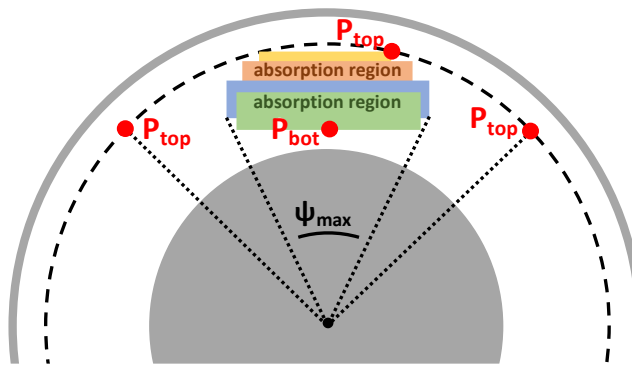


Figure 5.1: Cross section of a transiting exoplanet, with the host star on the left and the observer on the right. The grey disk represents the planetary interior, while the white annulus is the atmosphere of the planet. **(A)** For a stellar light ray with a particular impact parameter $R + z_t$ (yellow arrow), the opening angle ψ can be computed from trigonometry, using the maximum pressure P_{bot} and minimum pressure P_{top} probed by the light ray. For pressures lower than P_{bot} , the atmosphere's impact on the transmission spectrum is negligible. **(B)** In reality, the absorption region probed by the observation at a particular wavelength is vertically extended, such that P_{bot} and P_{top} do not lie along the same transit chord. **(C)** The absorption regions associated with different wavelengths lie at different altitudes. The values of the highest P_{bot} and the lowest P_{top} can suggest a much larger opening angle than is truly the case.

atmospheric opacities have a “measurable” impact on the planet’s transmission spectrum (analogous to the TCF). The opening angle can then be defined as

$$\psi \equiv 2 \arccos \left(\frac{R_p}{R_p + z(P_{\text{top}})} \right), \quad (5.1)$$

with R_p the planetary radius at P_{bot} and $z(P_{\text{top}})$ the altitude at P_{top} . Assuming an isothermal atmosphere with variable gravity, the hydrostatic equation reads

$$\int_{P_{\text{bot}}}^{P_{\text{top}}} \frac{dP}{P} = - \int_0^{z(P_{\text{top}})} \frac{dz}{H} \left(\frac{R_p}{R_p + z} \right)^2, \quad (5.2)$$

where H is the scale height at R_p . Solving this equation yields

$$z(P_{\text{top}}) = \frac{R_p}{1 - \frac{H}{R_p} \ln \left(\frac{P_{\text{bot}}}{P_{\text{top}}} \right)} - R_p, \quad (5.3)$$

such that the opening angle becomes (Caldas et al. 2019)

$$\psi \equiv 2 \arccos \left(1 - \frac{H}{R_p} \ln \left(\frac{P_{\text{bot}}}{P_{\text{top}}} \right) \right). \quad (5.4)$$

This result demonstrates that the opening angle is mainly governed by the ratio between the scale height and the radius of the planet. The greater this ratio, the larger the opening angle and the greater the importance of the line-of-sight dimension. Based on arguments from the literature, Caldas et al. (2019) assumed $(P_{\text{bot}}, P_{\text{top}}) = (10^{-2}, 10^{-5})$ bar. They found that the opening angle of the hot Jupiter HD 209458 b can be expected to exceed 30 degrees, while that of the sub-Neptune GJ 1214 b lies in the order of 45–50 degrees.

Although equation 5.4 provides a quick and simple estimate for the opening angle, one downside is the assumption that the minimum and maximum pressure probed by the observation are situated along the same transit chord (top panel in Fig. 5.1). In this case, the triangle with P_{top} and P_{bot} as two of its vertices is right-angled. However, if we consider a particular wavelength, the absorption region does not only stretch along the line of sight, but also in the vertical direction. As shown in the middle panel of Fig. 5.1, the minimum and maximum pressure contained in this absorption region do not lie along the same transit chord. As a result, the opening angle that is found by plugging P_{bot} and P_{top} into equation 5.4 is larger than the actual angular extent of the absorption region. This effect is enhanced when we consider multiple wavelengths. In a transmission spectrum, the effective radius of the planet changes because the absorption region moves up and down with wavelength. Consequently, the overall highest P_{bot} and the overall lowest P_{top} probed by the observation lie even further apart compared to the single-wavelength case (because the pressures are not probed by the same wavelength). This is illustrated in the bottom panel of Fig. 5.1. Because P_{top} and P_{bot} lie on two different transit chords, the opening angle is overestimated.

5.3 A new formula for the opening angle

In this section, we revisit the opening angle introduced by [Caldas et al. \(2019\)](#) and we derive an alternative formula that does not contain P_{top} and P_{bot} . Up to equation 5.7, our approach is similar to the derivation presented in Section A.2 from [Caldas et al. \(2019\)](#). However, the authors do not explicitly solve for the opening angle of a uniform, 1D atmosphere, as we do in equation 5.10. Additionally, we use a radiative-transfer code to validate the new formula and explicitly reconstruct the absorption regions discussed in the previous sections.

5.3.1 Derivation

We consider an isothermal atmosphere with one absorbing species and a transit chord at a height z_t above the reference radius R_p . Under the assumption of a uniform composition and a constant gravity, the integrated optical depth τ at position x is given by (Appendix A in [Caldas et al. 2019](#)):

$$\tau(x, z_t) = \sqrt{2\pi R_p H} \sigma_{\text{mol}} \chi n_0 e^{-z_t/H} \left[\frac{1}{2} + \frac{1}{2} \text{erf} \left(\frac{x}{\sqrt{2R_p H}} \right) \right], \quad (5.5)$$

with τ and x increasing in the direction towards the observer and $x = 0$ in the limb plane. Additionally, σ_{mol} is the constant² cross-section of the considered species, χ is its number fraction, n_0 is the particle number density at the reference radius, and H is the atmosphere's constant scale height. The derivation of equation 5.5 also requires that $|z_t| \ll 2R_p$, such that the altitude at position x can be written as $z \approx z_t + x/2R_p$ ([Fortney 2005](#); [Caldas et al. 2019](#)). In other words, the distance between the transit chord and the reference radius should be much smaller than the reference radius itself.

When we integrate along the full transit chord, the total optical depth becomes

$$\tau_0(z_t) \equiv \tau(x \rightarrow \infty, z_t) = \sqrt{2\pi R_p H} \sigma_{\text{mol}} \chi n_0 e^{-z_t/H}. \quad (5.6)$$

This equation allows us to express the altitude associated with the transit chord as a function of its total optical depth τ_0 (see also [Lecavelier des Etangs et al. 2008](#)):

$$z_t(\tau_0) = H \ln \left(\sqrt{2\pi R_p H} \sigma_{\text{mol}} \chi n_0 / \tau_0 \right). \quad (5.7)$$

We now define β , the ratio between the optical depth at a certain position x and the total optical depth associated with the transit chord:

$$\beta(x) \equiv \frac{\tau(x, z_t)}{\tau_0(z_t)} = \frac{1}{2} + \frac{1}{2} \text{erf} \left(\frac{x}{\sqrt{2R_p H}} \right), \quad (5.8)$$

which is independent of z_t . Inverting this equation yields

$$x(\beta) = \sqrt{2R_p H} \text{erf}^{-1}(2\beta - 1). \quad (5.9)$$

²In reality, σ_{mol} is a function of pressure, temperature and wavelength.

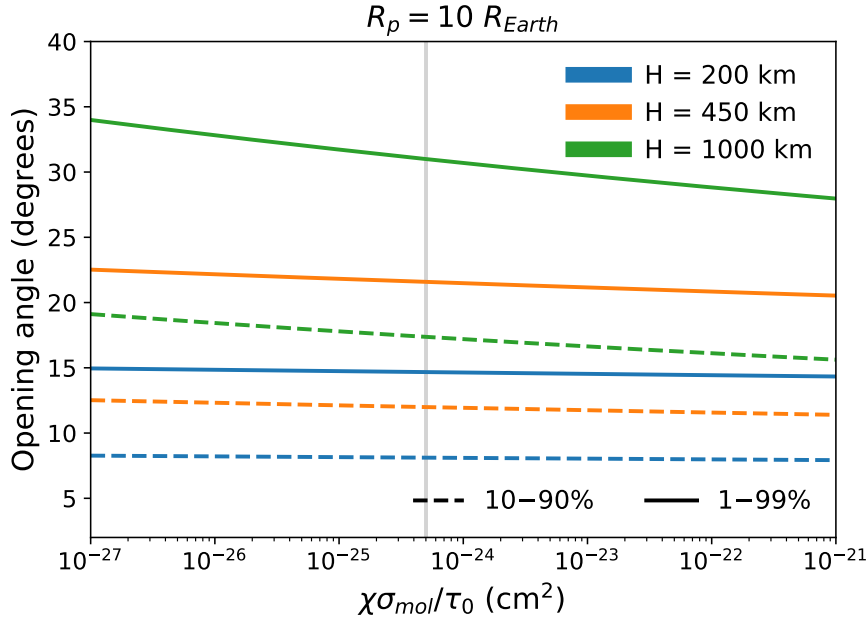


Figure 5.2: Plot of the analytical opening angle (equation 5.10) as a function of $\chi\sigma_{\text{mol}}/\tau_0$, for a planet with a radius of $10 R_{\text{Earth}}$. The figure shows the angles for three different scale heights and two values of β . Here, $\beta = 0.1$ corresponds to the 10–90% absorption region, while $\beta = 0.01$ gives rise to the 1–99% absorption region (see Section 5.3.2). The grey vertical line denotes the value of $\chi\sigma_{\text{mol}}/\tau_0$ that is used in this work. Also, we assume a constant gravity $g = 10 \text{ m/s}^2$ and mean molecular weight $\mu = 2.3 m_{\text{H}}$.

Using equations 5.7 and 5.9, we can now compute the opening angle associated with a transit-chord segment along which the optical depth increases from a fraction β to a fraction $(1 - \beta)$ of the total optical depth τ_0 :

$$\begin{aligned} \psi(\tau_0, \beta) &= 2 \arctan \left(\frac{|x(\beta)|}{R_p + z_t(\tau_0)} \right) \\ &= 2 \arctan \left(\frac{\sqrt{2R_p H} \operatorname{erf}^{-1}(1 - 2\beta)}{R_p + H \ln(\sqrt{2\pi R_p H} \sigma_{\text{mol}} \chi n_0 / \tau_0)} \right), \end{aligned} \quad (5.10)$$

with $\beta < 0.5$. The argument of the inverse error function was negated to get rid of the absolute-value symbols. To compute the opening angle subtended by an absorption region (i.e. the region of the atmosphere about which the transmission spectrum contains information), one can set $\tau_0 = 0.56$ (Lecavelier des Etangs et al. 2008). For a wide range of R_p/H values, a transit chord with this optical depth lies at an altitude z_t such that a fully opaque disk with radius $R_p + z_t$ would give rise to the same transit depth as the planet. About 43% of the light is absorbed along a transit chord with $\tau_0 = 0.56$.

Fig. 5.2 illustrates the dependence of the analytical opening angle on the assumed (constant) cross-section and abundance of the absorbing species. Because of the logarithmic dependence, the opening angle does not drastically change when $\chi\sigma_{\text{mol}}/\tau_0$ is varied over several orders of magnitude.

5.3.2 Numerical verification

Atmospheric models and radiative transfer

To verify whether equation 5.10 produces the correct values for ψ (given all the simplifying assumptions), we set up 1D isothermal atmospheres for 27 combinations of scale height $H \in \{10, 40, 90, 200, 450, 1000\}$ km and planetary radius $R_p \in \{1, 2, 5, 10, 20\} R_{\text{Earth}}$. For each (H, R_p) combination, we assume a constant gravity $g = 10 \text{ m/s}^2$ and mean molecular weight $\mu = 2.3 m_{\text{H}}$. In accordance with [Caldas et al. \(2019\)](#), we define the planetary radius to coincide with $P = 0.01$ bar. The atmospheres have 100 vertical layers, over which the pressure drops from $P = 10$ bar (bottom) to $P = 10^{-8}$ bar (top). Additionally, the (equivalent) temperature of the atmospheres follows from $T = \mu H g / k_B$, with k_B the Boltzmann constant. The particle number density at the reference radius, n_0 , follows from the ideal gas law.

In each model, we assume that there is one absorber with a constant abundance and cross-section, such that $\chi \sigma_{\text{mol}} / \tau_0 = 10^{-24.3} \text{ cm}^2$ (corresponding to e.g., $\chi = 10^{-3.3}$, $\sigma_{\text{mol}} = 10^{-21.3} \text{ cm}^2$ and $\tau_0 = 0.56$). These values are typical for an atmosphere with H_2O and/or CO at a solar abundance level (e.g., [Venot & Agúndez 2015](#); [Line et al. 2021](#)), but they could represent any chemical species – whichever one turns out to be the dominant absorber. In Fig. 5.2, we show that the dependence of the opening angle on $\chi \sigma_{\text{mol}} / \tau_0$ is relatively weak (because of the logarithm in equation 5.10), so a rough estimate suffices. On the other hand, changing the value of β has a much bigger effect on the opening angle.

Once all atmospheric models have been obtained, we compute their absorption regions. To this end, we use HIRES-CMCRT (see Chapters 2 and 4), a high-resolution version of the cloudy Monte-Carlo radiative transfer code (CMCRT) developed by [Lee et al. \(2017, 2019\)](#). Since the opacity of the atmospheres is constant, their transmission spectrum is flat and it suffices to compute the absorption region at a single wavelength point. For the purposes of this chapter, we use HIRES-MCRT as a 2D code, where we only illuminate the equatorial plane of the planet. We initialise 10^5 photon packets with a random impact parameter $R_p + z_t \in (R_p + z_{\text{min}}, R_p + z_{\text{max}})$, where $z_{\text{min}} < 0$ and $z_{\text{max}} > 0$ are the altitudes at the bottom and the top of the atmosphere, respectively. For each photon packet, we evaluate the optical depth along its transit chord in a polar geometry, with 100 vertical levels and 128 longitude slices. That is,

$$\tau_0(z_t) = \chi \sigma_{\text{mol}} \sum_{i=1}^{N_{\text{cells}}} n_i \Delta x_i, \quad (5.11)$$

with n_i the particle number density in the i -th atmospheric cell and Δx_i the distance the photon packet travels through this cell.

Constructing absorption regions

In addition to equation 5.11, we also keep track of the optical depth encountered by a photon packet as a function of position. Using this information, we can reconstruct the absorption regions of the atmosphere. For a given value of β (see equation 5.10), we define the absorption region in two steps. Firstly, we select all transit chords for which the total transmission $e^{-\tau_0}$ ranges between β and $1 - \beta$. Secondly, for each transit chord from the first step, we select the segment along which the optical depth increases from $\beta \tau_0$ to $(1 - \beta) \tau_0$. All segments

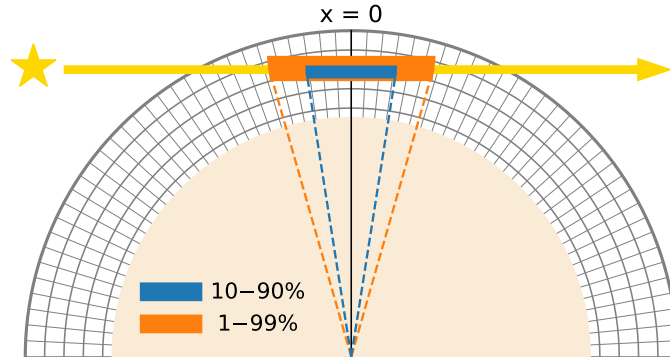


Figure 5.3: 10–90% and 1–99% absorption regions for the grey atmosphere with $R_p = 10 R_{\text{Earth}}$ and $H = 1000$ km, computed with HIRES-MCRT. The limb of the planet is indicated by $x = 0$, while the yellow arrow represents a stellar light ray crossing the atmosphere. The grey circles represent isobars of 1, 10^{-2} , 10^{-4} , 10^{-6} and 10^{-8} bar (in reality, the models have 100 pressure layers). The dashed lines show the opening angles associated with both absorption regions. The atmosphere and the planet are to scale in this figure.

together constitute the absorption region.³ We compute absorption regions for $\beta = 0.01$ and $\beta = 0.1$, which will be referred to as the 1–99% and 10–90% absorption regions in the rest of this chapter.

Fig. 5.3 shows the absorption regions for the model with $R_p = 10 R_{\text{Earth}}$ and $H = 1000$ km. The 10–90% region is fully contained by the 1–99% region, in agreement with the definition. Once the absorption regions are computed, their corresponding opening angle ψ_{abs} can be found geometrically (see Fig. 5.3):

$$\psi_{\text{abs}} = 2 \arctan \left(\frac{\bar{x}}{2\bar{y}} \right), \quad (5.12)$$

with $\bar{x}$ the average length of the segments in the absorption region and $\bar{y}$ the average distance of the segments from the centre of the planet. equation 5.12 holds as long as the absorption region is symmetric about the limb plane.

Comparing the formula to the model

Fig. 5.4 shows the opening angles computed from equation 5.12 for each of the 27 atmospheric models. For both values of β , there is a good agreement between the analytical opening angle from equation 5.10 (colour map) and the opening angle inferred from the absorption regions computed with the Monte-Carlo code (values in grey circles). It should be noted that the *analytical* opening angle is only based on the transit chord with $\tau_0 = 0.56$, while the opening angles associated with the absorption regions are based on all transit chords with $\beta < e^{-\tau_0} < 1 - \beta$. This may explain slight differences in Fig. 5.4 towards higher values of ψ .

³For instance, when $\beta = 0.1$, the absorption region includes all transit chords for which $0.1 < e^{-\tau_0} < 0.9$. Additionally, we only select the segment of every transit chord where the optical depth increases from 10% to 90% of its final value, such that the absorption region does not stretch all the way to the (arbitrary) model boundaries. By construction, the absorption region is symmetric about the limb plane in the limit of a 1D, uniform atmosphere.

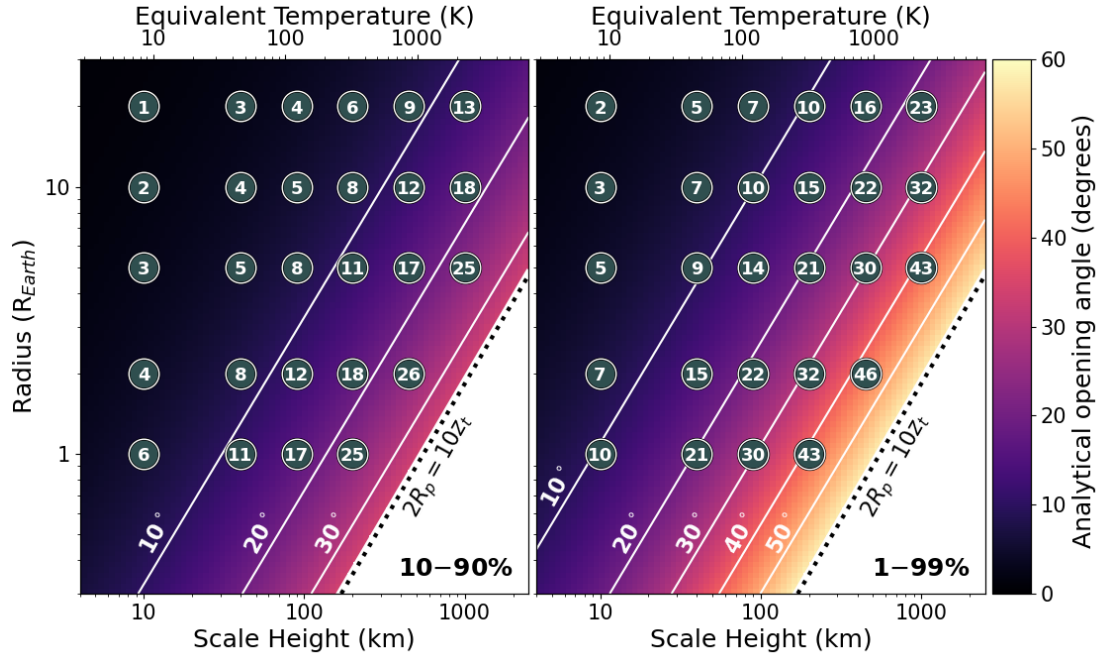


Figure 5.4: Colour maps showing the opening angle from equation 5.10 as a function of scale height H and planetary radius R_p , for $\beta = 0.1$ (left panel, 10–90% absorption) and $\beta = 0.01$ (right panel, 1–99% absorption). Additionally, we used $\chi\sigma_{\text{mol}}/\tau_0 = 10^{-24.3} \text{ cm}^2$. In the region to the right of the dotted lines, the approximation $|z_t| \ll 2R_p$ starts to break down, and hence it was excluded from the map. The values in the grey circles denote the opening angles (in degrees) that were geometrically calculated from the Monte-Carlo radiative transfer.

The trends in Fig. 5.4 are very similar to those in Fig. 2 from Caldas et al. (2019). The value of the opening angle increases as a function of the ratio H/R_p , which is in agreement with equation 5.4. Furthermore, the plots illustrate how the value of β impacts the opening angle. For the largest scale heights, the 1–99% opening angles are a factor ~ 1.8 bigger than the 10–90% opening angles. This is because with increasing β , a longer segment of the transit chord is included in the absorption region. In Section 5.5, we will investigate which value of β yields a realistic estimate for the true opening angle of a planet.

5.4 The wavelength dependence of the opening angle

In reality, planet atmospheres do not have a constant opacity. In this section, we examine how the opening angle changes when we account for the fact that σ_{mol} is a function of pressure, temperature and wavelength.

5.4.1 Atmospheric models and radiative transfer

We set up 27 atmospheric models with the same parameters as those described in Section 5.3.2. This time, however, we assume a variable gravity ($g = 10 \text{ m/s}^2$ at the reference radius), in accordance with the formula from Caldas et al. (2019). Furthermore, we include the chemical species H_2 , He , H_2O and CO , with number fractions $\chi_{\text{H}_2} = 0.76$, $\chi_{\text{He}} = 0.24$, $\chi_{\text{H}_2\text{O}} = 10^{-3.3}$ and $\chi_{\text{CO}} = 10^{-3.3}$. Again, we use HIRES-MCRT as a 2D code to compute the

absorption regions and transit spectra associated with the models. We account for the opacities of H₂O (Polyansky et al. 2018) and CO (Li et al. 2015), taken from the ExoMol database (Tennyson et al. 2016, 2020), as well the continuum due H₂-H₂ and H₂-He collision-induced absorption (Borysow et al. 2001; Borysow 2002; Gordon et al. 2017). The radiative transfer is performed at high spectral resolution ($R = 500,000$), for 213 wavelength points near 2.34 micron (see Fig. 5.5). The rationale behind this approach is that at high resolution, cross-sections vary dramatically as a function of wavelength – depending on whether λ lies inside or outside a line core. Therefore, modelling the atmospheric absorption around just a number of line cores should already produce a spectrum that probes many different atmospheric layers.

Because the cross-sections are no longer constant, we now evaluate the optical depth along a transit chord as:

$$\tau_0(z_t, \lambda) = \sum_{i=1}^{N_{\text{cells}}} n_i \Delta x_i \left[\sum_{j=1}^{N_{\text{species}}} \chi_j \sigma_{\text{mol},i,j}(\lambda) \right], \quad (5.13)$$

with χ_j the number fraction of the j -th species and $\sigma_{\text{mol},i,j}$ its cross-section in the i -th atmospheric cell. Once the optical depth is computed along all transit chords, the effective area $A_{\text{eff}}(\lambda)$ of the planet can be found from (see also Chapter 2)

$$A_{\text{eff}}(\lambda) = A_0 + A_{\text{annu}} \langle 1 - e^{-\tau} \rangle_{\lambda}, \quad (5.14)$$

with A_0 the projected area of the planetary interior and A_{annu} the area of the atmospheric annulus. The angle brackets denote an average over all photon packets with wavelength λ .

5.4.2 Results

The bottom panel of Fig. 5.5 shows the 10–90% and 1–99% opening angles obtained for the model with $R_p = 10 R_{\text{Earth}}$ and $H = 450$ km (solid curves). These were computed from the absorption regions using equation 5.12. Because of the wavelength-dependence of the opacities, the opening angle is no longer constant and tends to acquire its highest values inside a line core. This may seem counter-intuitive, because according to equation 5.10, the opening angle is a monotonically decreasing function of σ_{mol} . However, the solid curves show the opening angle associated with absorption regions that have the *same* values of τ_0 (i.e. $\tau_0 \sim 0.56$), regardless of the wavelength. Consider two wavelengths λ_1 and λ_2 with opacities $\sigma_1(P_A) > \sigma_2(P_A)$ at a certain pressure P_A . If the absorption region of λ_2 lies around P_A , the absorption region of λ_1 will lie around some pressure $P_B < P_A$, higher up in the atmosphere. To compute the opening angle at λ_1 , we must hence plug $\sigma_1(P_B)$ – which is potentially smaller than $\sigma_2(P_A)$ – into equation 5.10.

The dotted curves in the same panel show the result of evaluating the Caldas et al. (2019) formula (equation 5.4) using the highest pressure (P_{bot}) and the lowest pressure (P_{top}) contained by the absorption region at a particular wavelength (see middle panel of Fig. 5.5). As illustrated in the middle panel of Fig. 5.1, this leads to an overestimation of the opening angle, because P_{bot} and P_{top} do not lie on the same transit chord. Alternatively, if one applies equation 5.4 to every *individual* transit chord in the absorption region and takes an average (dashed curves), the Caldas et al. (2019) formula and the radiative-transfer model agree very well. This result demonstrates that P_{top} and P_{bot} should not be chosen by looking at

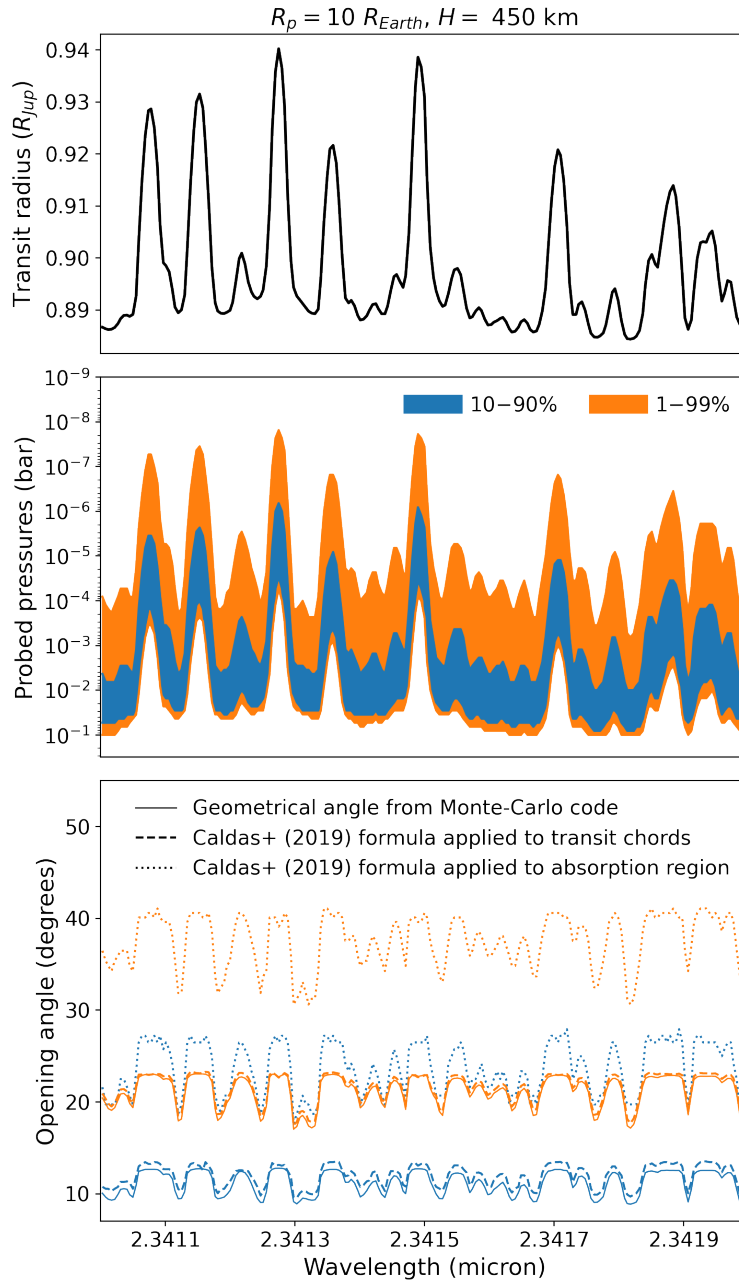


Figure 5.5: Radiative-transfer output for the model with $R_p = 10 R_{\text{Earth}}$ and $H = 450$ km. **Top:** The transmission spectrum, featuring H_2O and CO absorption lines. **Middle:** The pressures contained by the 10–90% and 1–99% absorption regions as a function of wavelength. **Bottom:** The 10–90% and 1–99% opening angles as a function of wavelength. The solid curves were obtained using the method described in section 5.3.2. The dashed curves show the output of the Caldas et al. (2019) formula when the P_{bot} and P_{top} of *individual* transit chords are plugged into the formula, while the dotted curves illustrate what happens when the P_{bot} and P_{top} of the full absorption region are used (as depicted in the middle panel of Fig. 5.1). The latter leads to an overestimation of the opening angle.

the $\tau_0 \sim 0.56$ level corresponding to the lowest and highest opacity values in the considered bandpass.

As far as the other models are concerned, we note that for all atmospheres with $H \leq 200$ km, the standard deviation in the opening angle with wavelength is 10 to 15% of the mean value. For models with $H = 450$ km and large planetary radii, the relative spread drops to 7%. Atmospheres with the largest scale height exhibit a very small spread in their opening angle with wavelength, below 2%.

5.5 Opening angles and instrument noise

In order to make a final, proper comparison between the [Caldas et al. \(2019\)](#) formula (equation 5.4) and our newly derived formula for the opening angle (equation 5.10), we need to determine what value of β is appropriate when estimating the opening angle of an atmosphere. After all, picking a larger value for β results in larger values for the opening angle $\psi(\tau_0, \beta)$. As discussed in the Section 5.2, the opening angle should be defined such that the opacities *outside* the corresponding absorption region do not have a “measurable” impact on the transmission spectrum of the planet. Strictly speaking, this means that the opening angle is not just dependent on the atmospheric structure, but also on the telescope or instrument through which the planet is observed. In this section, we will assume an instrument noise floor of 10 ppm, roughly comparable to that of JWST ([Beichman et al. 2014](#); [Schlawin et al. 2021](#)).

5.5.1 Atmospheric models and radiative transfer

For each model from Section 5.4.1, we now seek to determine the number of longitude slices to which an observation with a 10-ppm noise floor is actually sensitive. Unlike [Lacy & Burrows \(2020\)](#), we do not switch off the opacities of *individual* longitude slices (see Section 5.6.1 for further discussion). Instead, for each model, we calculate 31 new spectra, where we only preserve the opacities inside the $2n$ longitude slices that are closest to the terminator (with $n = 1, 2, 3, \dots, 31$). The opacities in all the other slices are set to zero. Fig. 5.6 shows what the equatorial plane of the planet looks like when different numbers of longitude slices⁴ are “activated”. Of course, the spectra of the models should converge to the true spectrum of the planet (i.e. $n = 32$) as n increases. To obtain the final transmission spectra, we assume a stellar radius of one solar radius. Once all spectra are computed, we determine the difference between the wavelength-averaged transit depth of the 31 models and that of the full atmosphere ($n = 32$). We then define the opening angle (in degrees) as the smallest value of $(360/64)n$ for which this difference lies below 10^{-5} .

5.5.2 Results

The top panel of Fig. 5.7 depicts the transmission spectra of the models with $R_p = 10 R_{\text{Earth}}$ and $H = 1000$ km. As more longitude slices are activated in the models, the transit depth of the planet increases. At some point, however, the atmospheric width is such that the spectrum can no longer be distinguished from the spectrum of the full atmosphere. The bottom panel of Fig. 5.7 shows the wavelength-averaged difference between the transit depths of

⁴Each longitude slice has an angular width of $360/128 \approx 2.8$ degrees.

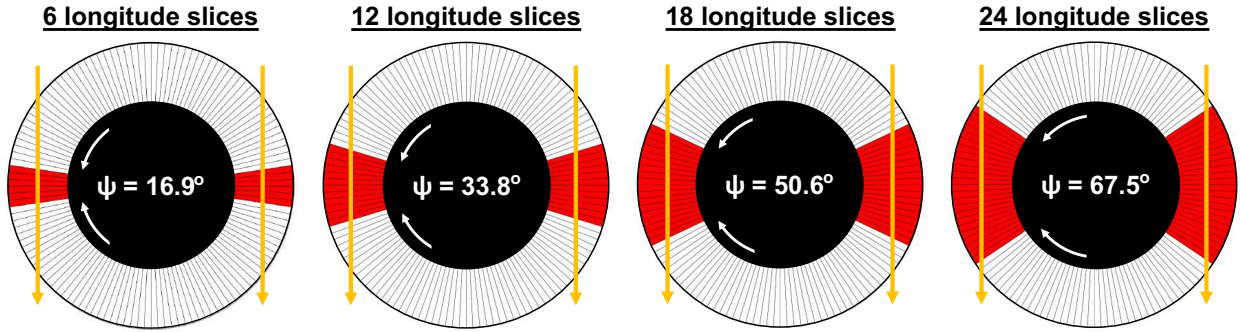


Figure 5.6: The equatorial plane of four model atmospheres, where we only preserve the opacities within a certain angle from the terminator (red area). The opacities of the other longitude slices are set to zero (white area). The yellow arrows represent stellar light rays pointing towards the observer. ψ is the angular width of the atmosphere.

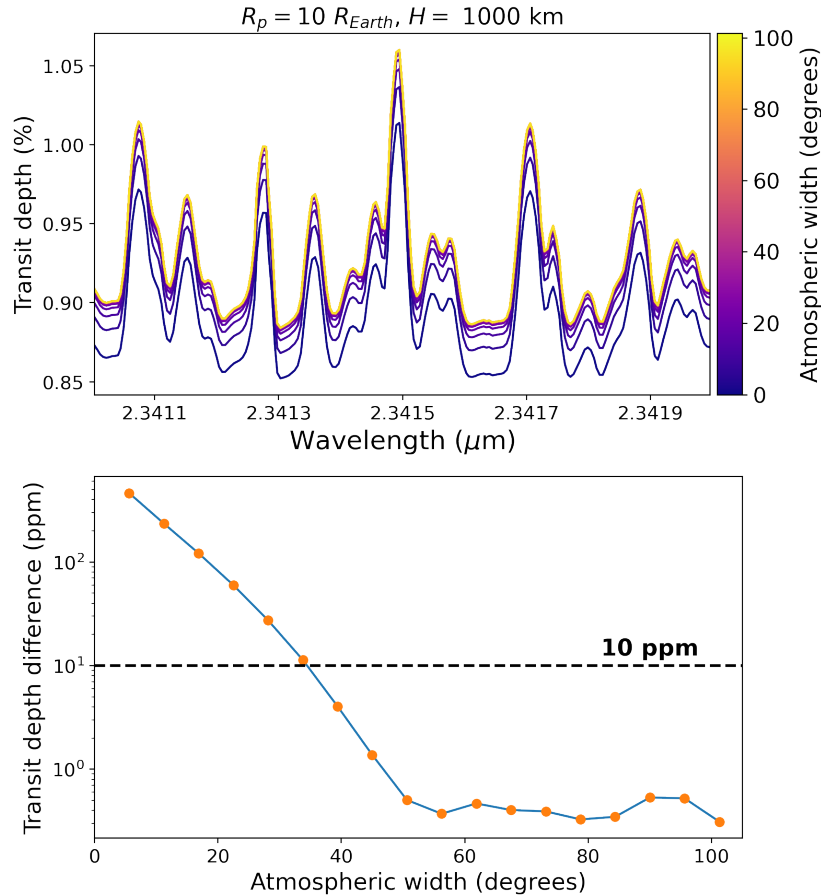


Figure 5.7: Radiative-transfer output for the atmosphere with $R_p = 10 R_{\text{Earth}}$ and $H = 1000$ km. **Top:** Transmission spectra for models with a different number of activated longitude slices and, therefore, a different atmospheric width. **Bottom:** The wavelength-averaged difference between the transit depth of the models (orange markers) and the transit depth of the full atmosphere, in which none of the opacities are set to zero.

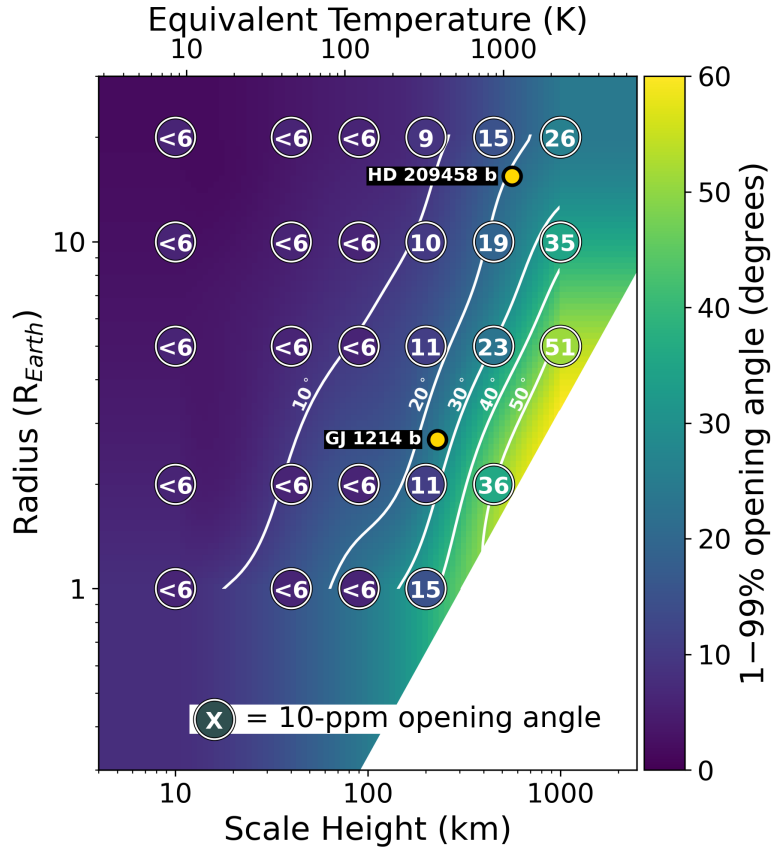


Figure 5.8: Opening angles as a function of scale height and planetary radius. The circles contain the opening angles found from the method described in Section 5.5.1, where we assume a 10-ppm noise floor. The colour map in the background shows the 1–99% opening angles (averaged over all wavelengths from Section 5.4) and was obtained from interpolation. Contour lines are shown in white.

the models (orange markers) and the full atmosphere. For this particular combination of planetary radius and scale height, the opening angle is 35 degrees, because models with a larger atmospheric width cannot be distinguished from the full atmosphere above the 10 ppm level. Because of the stochastic nature of the Monte-Carlo code, the simulations also have their own noise floor (below 1 ppm), which is why the curve in the bottom panel does not continue to decrease.

The circles in Fig. 5.8 show the 10-ppm opening angles obtained for all the 27 models considered in this work. For all atmospheres with a scale height $H \leq 90$ km, the opening angle is smaller than 6 degrees, because the difference between the spectrum of the $n = 1$ model and that of the full atmosphere is already smaller than 10 ppm. In other words, given a noise floor of 10 ppm, one cannot distinguish between the full planet atmosphere and a model with an atmospheric width of only 6 degrees. Therefore, if we want to make a comparison between the opening angles found from the absorption regions (Section 5.4) and those based on the 10-ppm noise floor (this section), we need to focus on the atmospheres with the largest scale heights and planetary radii – see the top right corner of Fig. 5.8.

For $R \geq 5 R_{\text{Earth}}$ and $H \geq 200$ km, the opening angles corresponding to the 1–99% absorption regions are in relatively close agreement with the opening angles obtained from the 10-ppm noise floor. On the other hand, the 10–90% opening angles (not shown in the figure)

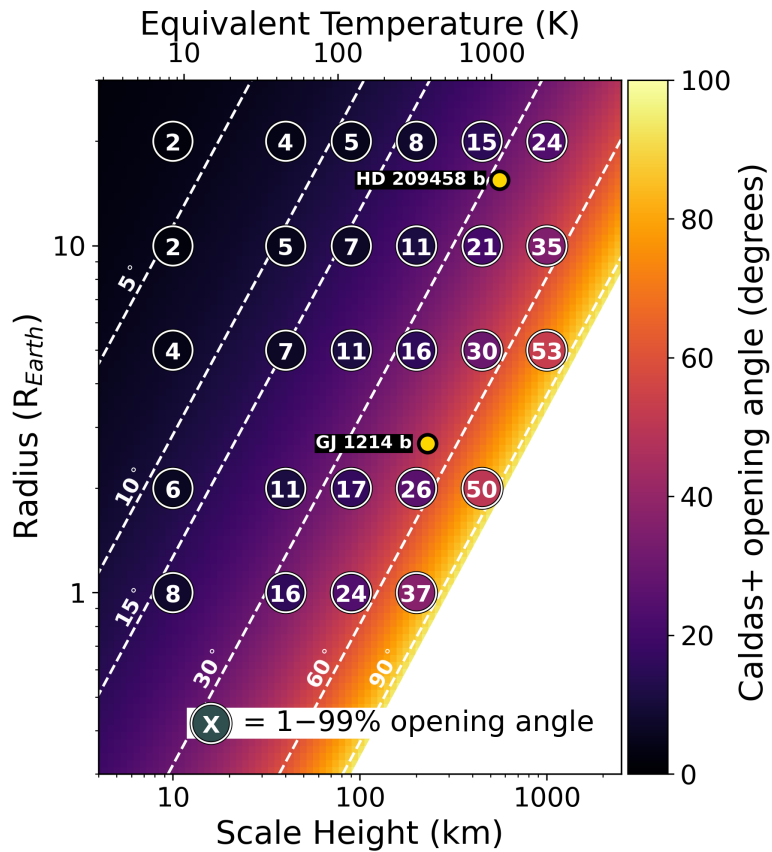


Figure 5.9: Opening angles as a function of scale height and planetary radius. The circles contain the 1–99% opening angles found for all 27 models considered in this work (Section 5.4). The colour map in the background shows the opening angles that follow from the [Caldas et al. \(2019\)](#) formula, assuming $(P_{\text{bot}}, P_{\text{top}}) = (10^{-2}, 10^{-5})$ bar. Contour lines are shown in white dashes.

are too small to match these values. Based on the models presented here, this suggests that $\beta = 0.01$ is an appropriate value to plug into equation 5.10 when making an estimate of an atmosphere’s opening angle – at least when $R \geq 5 R_{\text{Earth}}$ and $H \geq 200$ km. This is also the regime where most planets with currently known radii and scale heights reside ([Caldas et al. 2019](#)). For smaller planetary radii, the 10-ppm opening angles are smaller than those derived from the 1–99% absorption region. Hence, the latter can be seen as an upper limit.

5.6 Discussion

5.6.1 Comparison to previous works

In this chapter, we derived a formula for the opening angle as a function of opacity and optical depth, instead of the bottom pressure P_{bot} and top pressure P_{top} probed by a transit observation. This approach is advantageous, because it can be hard to pick values for P_{bot} and P_{top} such that they lie on the same transit chord. As shown in Fig. 5.5, the [Caldas et al. \(2019\)](#) formula (equation 5.4) is correct when applied to a single transit chord. However, when the maximum and minimum pressure probed across a bandpass are plugged into the formula, the opening angle can be strongly overestimated. This is demonstrated in Fig. 5.9.

The discrepancy is biggest for planets with small radii and large scale heights.

In contrast to our study, [Lacy & Burrows \(2020\)](#) did find a good agreement between their computed opening angles and the [Caldas et al. \(2019\)](#) formula (see their Fig. 4). Using a 3D radiative-transfer model, the authors applied the same technique as [Mollière et al. \(2019\)](#) to compute the TCF as a function of longitude. That is, instead of perturbing the opacities across different altitudes, they set the opacities of individual longitude slices⁵ equal to zero, and evaluated the difference between the resulting spectrum and the spectrum of the full atmosphere. However, from their work, it is not clear how many longitude slices the authors used, what threshold⁶ (noise floor) they assumed, and how this impacted their results. After all, by lowering the noise floor (i.e. increasing the sensitivity of the instrument), one can always obtain larger values for the opening angle (see Fig. 5.7).

5.6.2 Implications of this study

The fact that we find smaller opening angles compared to [Caldas et al. \(2019\)](#) and [Lacy & Burrows \(2020\)](#) does not mean that 3D modelling becomes less important in the context of retrievals. We find opening angles in the order of 20–25 degrees for (ultra-)hot Jupiters, and this is still a big number compared to the angle over which thermal and chemical gradients can occur. [Caldas et al. \(2019\)](#), [Pluriel et al. \(2020, 2021\)](#), for example, present models in which the transition from dayside to nightside chemistry spans less than 10 degrees (see also Chapters 4 and 6). Hence, these variations should still be taken into account when interpreting observational data. For cooler planets with smaller opening angles and gradients that are less steep, 1D modelling may be adequate.

In general, when dealing with variations along the line of sight, it will not be necessary for retrieval models to account for the full 360-degree structure of the atmosphere. Instead, it suffices to have a model that is as wide as the opening angle in the dimension orthogonal to the limb plane. Any opacities outside the opening angle have a negligible effect on the transmission spectrum of the planet.

As discussed in the introduction, absorption regions can be interpreted as (spatial) resolution elements. In the context of tidally locked gas giants, a smaller opening angle allows for (more) independent measurements in and around the equatorial plane of the planet. Fig. 5.10 shows the rotation angle of a planet as a function of its equilibrium temperature T_{eq} and the effective temperature T_{eff} of the host star, assuming it is tidally locked (see next section for the relevant equations). The rotation angle is the angle over which the planet rotates during its transit. Given a certain planet radius, there exists a curve connecting all $(T_{\text{eq}}, T_{\text{eff}})$ points for which the rotation angle of the planet is equal to its opening angle. To the right of this curve, the rotation angle is *larger* than the opening angle. As shown in Fig. 5.10, the curve shifts to higher T_{eq} values when the planet radius is smaller (red vs yellow). The selected value of β impacts the curve in a similar way (solid vs dashed). According to Fig. 5.10, however, ultra-hot Jupiters such as WASP-76b, WASP-121b and KELT-9b all have rotation angles that are larger than their (1–99%) opening angles. In the *equatorial plane*, this means

⁵Technical note (private communication): [Lacy & Burrows \(2020\)](#) rotated their 3D grid such that its poles coincided with the substellar and antistellar point of the planet. In this way, the latitude slices effectively take on the role of longitude slices, with the benefit that they are equally thick across the entire atmospheric annulus (i.e. there is no singularity at the geographical poles).

⁶[Lacy & Burrows \(2020\)](#) refer to a “non-zero change in the transit spectrum”, which suggests an arbitrarily low noise floor.

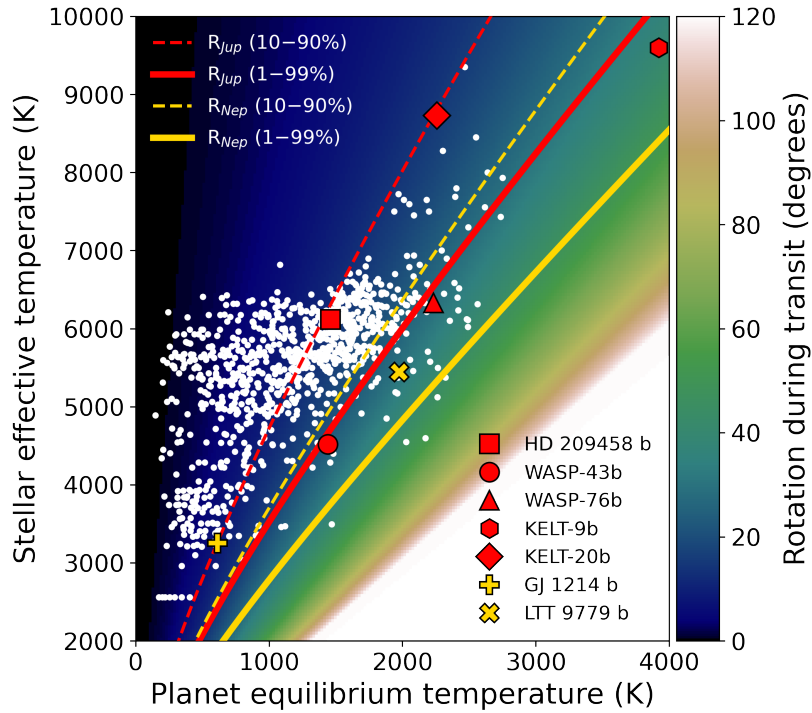


Figure 5.10: The angle over which a tidally locked planet rotates during its transit, plotted as a function of its equilibrium temperature T_{eq} (assuming zero albedo and full heat redistribution) and the effective temperature T_{eff} of the host star. The white bullets show all systems for which the stellar radius and the semi-major axis of the planet orbit are currently known (data acquired from <https://www.astro.keele.ac.uk/jkt/tepcat/>; Southworth 2011). The red and yellow curves show for which $(T_{\text{eq}}, T_{\text{eff}})$ the planet’s rotation angle is equal to the opening angle. Here, we assume two different planet radii (one Jupiter radius and one Neptune radius), and two different values for β (see equation 5.10). To the right of the curves, the rotation angle is larger than the opening angle.

that the transit observation probes a completely different atmospheric region at the start of the transit than at the end of the transit. Consequently, measurements of the equatorial jet speed (Louden & Wheatley 2015; Showman & Polvani 2011) at the start and the end of the transit can be expected to be fully independent. Such observations would allow for further insights into the atmospheric circulation of (ultra-)hot Jupiters.

Derivation of Fig. 5.10

In Fig. 5.10, we plotted the planet’s rotation angle (assuming tidal locking and an edge-on orbit) as a function of its equilibrium temperature T_{eq} and the effective temperature T_{eff} of the host star. In what follows, we briefly present the equations behind the colour map and the curves that indicate where the rotation angle is equal to the opening angle.

For a tidally locked planet, the rotation angle ψ_{rot} is given by

$$\psi_{\text{rot}} = 2 \arcsin (R_{\star}/a), \quad (5.15)$$

with $R_{\star}$ the radius of the host star and a the semi-major axis. Because equation 5.15 does not contain the planet radius, it gives the rotation angle between the middle of the ingress and the middle of the egress.

Assuming zero albedo and full heat redistribution, the equilibrium temperature of the planet is

$$T_{\text{eq}} = T_{\text{eff}} \sqrt{R_{\star}/2a}. \quad (5.16)$$

Solving for $R_{\star}/a$ and plugging the result into equation 5.15 yields

$$\psi_{\text{rot}} = 2 \arcsin \left(2 (T_{\text{eq}}/T_{\text{eff}})^2 \right). \quad (5.17)$$

Also, this means that the effective temperature of the host star can be written as

$$T_{\text{eff}}(\psi_{\text{rot}}) = T_{\text{eq}} / \sqrt{\sin(\psi_{\text{rot}}/2)/2} \quad (5.18)$$

To compute where the rotation angle is equal to the opening angle, we take three steps. First, we choose a planet radius R_{p} . Next, we use equation 5.10 to compute the opening angle ψ_{open} as a function of T_{eq} . The opening angle depends on the equilibrium temperature through the scale height H . Furthermore, we assume the same parameter values as in Section 5.3.2. That is, $g = 10 \text{ m/s}^2$, $\mu = 2.3 m_{\text{H}}$ and $\chi\sigma_{\text{mol}}/\tau_0 = 10^{-24.3} \text{ cm}^2$. Finally, we use equation 5.18 to compute $T_{\text{eff}}(\psi_{\text{rot}} = \psi_{\text{open}})$.

5.7 Conclusion

We summarize our most important findings below:

- We derived and validated a new formula for the opening angle (equation 5.10) in the limit of a uniform atmosphere with constant gravity. It does not depend on P_{bot} and P_{top} , the maximum and minimum pressure probed by the transmission spectrum. Instead, the formula depends on the product $\sigma_{\text{mol}}\chi/\tau_0$, with σ_{mol} the constant cross-section of the considered species and χ its number fraction. τ_0 is the total optical depth of a transit chord that crosses the absorption region (typically, $\tau_0 = 0.56$).
- The opening angles of the absorption regions computed with our Monte-Carlo radiative transfer code (HIRES-MCRT) agree with the new formula (equation 5.10) in the limit of a grey, uniform atmosphere with constant gravity.
- When we account for the pressure, temperature and wavelength dependence of the cross-sections, we find that the opening angle acquires its maximum value inside a line core.
- The [Caldas et al. \(2019\)](#) formula (equation 5.4) results in an overestimation of the opening angle when P_{bot} and P_{top} of an absorption region are used. However, when the formula is applied to individual transit chords, it matches the angular extent of the absorption regions very closely.
- The β parameter in equation 5.10 governs what segment of the transit chord is subtended by the opening angle. Based on the models presented in this work, we find

that $\beta = 0.01$ is a good default choice. The resulting opening angle is the 1–99% opening angle, which corresponds to segment along which the optical depth increases from 1% to 99% of τ_0 .

- When we take instrument noise into account (assuming a noise floor of 10 ppm), we find that the opening angle is only bigger than a few degrees for hot planets, with a scale height larger than 100 km.
- For ultra-hot Jupiters, the typical angle over which the planet rotates during the transit is larger than the opening angle. This implies that measurements of the equatorial jet speed at the start and the end of the transit are fully independent.

Bibliography

- Arcangeli J., et al., 2018, *ApJ*, **855**, L30
- Barstow J. K., Aigrain S., Irwin P. G. J., Bowles N., Fletcher L. N., Lee J. M., 2013, *MNRAS*, **430**, 1188
- Beichman C., et al., 2014, *PASP*, **126**, 1134
- Bell T. J., Cowan N. B., 2018, *ApJ*, **857**, L20
- Borsa F., et al., 2021, *A&A*, **645**, A24
- Borysow A., 2002, *A&A*, **390**, 779
- Borysow A., Jørgensen U. G., Fu Y., 2001, *J. Quant. Spectrosc. Radiative Transfer*, **68**, 235
- Bourrier V., et al., 2020, *A&A*, **635**, A205
- Burrows A., Rauscher E., Spiegel D. S., Menou K., 2010, *ApJ*, **719**, 341
- Caldas A., Leconte J., Selsis F., Waldmann I. P., Bordé P., Rocchetto M., Charnay B., 2019, *A&A*, **623**, A161
- Charbonneau D., Brown T. M., Noyes R. W., Gilliland R. L., 2002, *ApJ*, **568**, 377
- Ehrenreich D., et al., 2020, *Nature*, pp 1–7
- Fortney J. J., 2005, *MNRAS*, **364**, 649
- Fortney J. J., Shabram M., Showman A. P., Lian Y., Freedman R. S., Marley M. S., Lewis N. K., 2010, *ApJ*, **709**, 1396
- Gordon I. E., et al., 2017, *J. Quant. Spectrosc. Radiative Transfer*, **203**, 3
- Hoeijmakers H. J., et al., 2020, *A&A*, **641**, A120
- Kesseli A. Y., Snellen I. A. G., 2021, *ApJ*, **908**, L17
- Lacy B. I., Burrows A., 2020, *ApJ*, **905**, 131
- Lecavelier des Etangs A., Pont F., Vidal-Madjar A., Sing D., 2008, *A&A*, **481**, L83
- Lee E. K. H., Wood K., Dobbs-Dixon I., Rice A., Helling C., 2017, *A&A*, **601**, A22
- Lee E. K. H., Taylor J., Grimm S. L., Baudino J.-L., Garland R., Irwin P. G. J., Wood K., 2019, *MNRAS*, **487**, 2082
- Li G., Gordon I. E., Rothman L. S., Tan Y., Hu S.-M., Kassi S., Campargue A., Medvedev E. S., 2015, *ApJ Supplement Series*, **216**, 15
- Line M. R., et al., 2013, *ApJ*, **775**, 137
- Line M. R., et al., 2021, *Nature*, **598**, 580
- Louden T., Wheatley P. J., 2015, *ApJ*, **814**, 1
- Mollière P., Wardenier J. P., van Boekel R., Henning T., Molaverdikhani K., Snellen I. A. G., 2019, *A&A*, **627**, A67
- Nikolov N., et al., 2018, *Nature*, **557**, 526
- Parmentier V., et al., 2018, *A&A*, **617**
- Pluriel W., Zingales T., Leconte J., Parmentier V., 2020, *A&A*, **636**, A66
- Pluriel W., Leconte J., Parmentier V., Zingales T., Falco A., Selsis F., Borde P., 2021, arXiv e-prints, p. [arXiv:2110.09080](https://arxiv.org/abs/2110.09080)
- Polyansky O. L., Kyuberis A. A., Zobov N. F., Tennyson J., Yurchenko S. N., Lodi L., 2018, *MNRAS*, **480**, 2597
- Schlawin E., et al., 2021, in American Astronomical Society Meeting Abstracts. p. 428.06
- Seager S., Sasselov D. D., 2000, *ApJ*, **537**, 916
- Showman A. P., Polvani L. M., 2011, *ApJ*, **738**, 71

- Sing D. K., et al., 2016, [Nature](#), 529, 59
- Snellen I. A. G., Albrecht S., de Mooij E. J. W., Poole R. S. L., 2008, [A&A](#), 487, 357
- Southworth J., 2011, [MNRAS](#), 417, 2166
- Tennyson J., et al., 2016, [Journal of Molecular Spectroscopy](#), 327, 73
- Tennyson J., et al., 2020, [J. Quant. Spectrosc. Radiative Transfer](#), 255, 107228
- Venot O., Agúndez M., 2015, [Experimental Astronomy](#), 40, 469
- Waldmann I. P., Tinetti G., Rocchetto M., Barton E. J., Yurchenko S. N., Tennyson J., 2015, [ApJ](#), 802, 107
- Wardenier J. P., Parmentier V., Lee E. K. H., 2022, [MNRAS](#), 510, 620

Chapter 6

The effect of 3D temperature and chemistry on the cross-correlation signal of transiting ultra-hot Jupiters: A study of 5 chemical species in WASP-76b

The material in this chapter is based on [Wardenier et al. \(2023\)](#):

– Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R. (submitted to MNRAS)

Abstract – Ultra-hot Jupiters are excellent targets for atmospheric characterisation in transmission. However, because these planets are tidally locked, their atmospheres feature strong spatial variations in temperature, chemistry, dynamics, cloud coverage, and scale height. This makes their high-resolution spectra difficult to interpret. In this work, we model the cross-correlation signal of five chemical species – Fe, CO, H₂O, OH, and TiO – in the atmosphere of WASP-76b, a benchmark ultra-hot Jupiter. Our 3D atmospheric models are based on outputs of the SPARC/MITgcm global circulation model. We use gCMCRT, a GPU-compatible Monte-Carlo radiative transfer code, to compute transmission spectra at different phases during the transit. From these spectra, we then obtain cross-correlation signals and K_p – V_{sys} maps to investigate how the 3D structure of ultra-hot Jupiters manifests in observations. We find that different chemical species have vastly different distributions, such that their absorption lines probe distinct regions of the atmosphere. Furthermore, we conclude that the day-night contrast of ultra-hot Jupiters consistently leads to increasing blueshifts for species that probe the dayside (e.g., all refractories), even if they are distributed uniformly across the atmosphere, like CO. This should remain true in the absence of an east-west asymmetry on the planet, such as a hotspot shift. Species probing the nightside can be subject to either an increasing or a decreasing blueshift. Finally, we show that our models yield systematic offsets in K_p – V_{sys} maps, whereby the K_p shift of a species can be much larger than its net Doppler shift at any orbital phase.

6.1 Introduction

As discussed in Chapter 3, “phase-resolving” the CCF of a transiting planet with sufficiently high accuracy is a challenge. To our knowledge, only the neutral iron (Fe or Fe I) signals of WASP-76b ([Ehrenreich et al. 2020](#)), WASP-121b ([Borsa et al. 2021](#)), and KELT-20b ([Rainer et al. 2021](#)) have been constrained at more than two orbital phases in transmission. For WASP-76b and WASP-121b, the CCFs show an increasing blueshift during the transit, with the peak position moving from about 0 km/s at ingress to about –10 km/s at egress. In the case of WASP-76b, multiple mechanisms were suggested for this behaviour, including iron condensation on the leading limb (Chapter 4; [Ehrenreich et al. 2020](#)), a scale-height difference between both limbs (Chapter 4), the presence of optically-thick clouds on the leading limb ([Savel et al. 2022](#)), or a combination of these effects. More recently, [Beltz et al. \(2023\)](#) proposed that the planet’s (spatially varying) magnetic field can also play a role. All in all, the interpretation of the ESPRESSO data is ambiguous, and more observations will be required to further constrain the atmospheric properties of WASP-76b and (ultra-)hot Jupiters

in general.

A good way forward would be to observe the phase-dependent absorption signals of species *other* than iron. With novel spectrographs such as GEMINI-S/IGRINS (Line et al. 2021; Mace et al. 2018) and VLT/CRIRES+ (Holmberg & Madhusudhan 2022; Dorn et al. 2023), it is now also possible to do this for molecules in the infrared, such as CO and H₂O. Moreover, once the E-ELT is on sky, phase-resolving the CCF will become standard practice for any high-resolution observation of a hot gas giant, as the signal-to-noise will be high enough to detect the planet in only a fraction of a transit. Also, the E-ELT will offer the opportunity to take ingress and egress spectra, whereby only a part of the planet disk is blocking the star. In ultra-hot Jupiters, observations of species in the optical and infrared are complementary, because they have distinct spatial distributions across the atmosphere. The CCFs of *different* species contain *different* pieces of information about the planet’s 3D temperature structure, its cloud cover, and its dynamics.

Phase-resolved observations are a powerful means to perform “local” measurements in an exoplanet atmosphere and obtain information about its 3D structure. For example, by dividing the ESPRESSO data from Ehrenreich et al. (2020) into two halves, Gandhi et al. (2022) were able to retrieve the temperature profile and iron abundance of WASP-76b at *four* different longitudes. Furthermore, they separately constrained the wind speeds on the trailing and leading limb of the planet. Performing similar retrieval studies in the infrared would be valuable for two reasons. Firstly, they allow to get a better handle on the planet’s “3D-ness”, as different species probe different atmospheric regions. Secondly, measuring the abundances of molecules such as CO, H₂O, and OH will allow to compute refractory-to-volatile ratios (e.g., Fe/O), which are important in the context of planet formation (see Chapter 1). However, the fact that the planet is 3D will render it more difficult to make these inferences. Therefore, we need 3D forward models to understand *how* 3D effects manifest in high-resolution spectra and *how* to best parameterise these effects in 1D or pseudo-2D models used in retrievals. Also, we require 3D forward models to understand what we can really learn from multi-species observations.

The aim of this chapter is to further explore the connection between the “3D-ness” ultra-hot Jupiters and their CCF signals in transmission. To this end, we build on earlier modelling work described in Chapter 4. We use gCMCRT to simulate phase-dependent transmission spectra for different atmospheric scenarios of WASP-76b, based on outputs of the SPARC/MITgcm. We then compute the CCF signals and K_p – V_{sys} maps for five different chemical species: Fe and TiO in the optical, and CO, H₂O, and OH in the infrared. The motivation for considering these species is that they all have *distinct 3D spatial distributions* across the planet. Therefore, the absorption lines associated with these species will probe different regions of the atmosphere, each with their own properties. Furthermore, the behaviour we identify for a certain species will be representative of other atoms and molecules with the same spatial distribution. For example, the signals we simulate for iron will be a good proxy for the signals of other refractories too.

The structure of this chapter is as follows. In Section 6.2 we describe our WASP-76b models, our radiative-transfer framework, and methods for computing CCF signals, K_p – V_{sys} maps and absorption regions. In Section 6.3, we present, discuss and interpret our results. Finally, Section 6.4 provides a conclusion.

Table 6.1: Overview of the four WASP-76b scenarios considered in this chapter, based on outputs of the SPARC/MITgcm.

Model	Drag time	Description
Nominal model	10^5 s	Nominal GCM output without post-hoc additions or modifications.
Cold morning limb	10^5 s	Nominal GCM output with modified thermochemical structure on the morning limb, following Chapter 4.
Optically thick clouds	10^5 s	Nominal GCM output with optically thick Al_2O_3 cloud added, following Savel et al. (2022).
No TiO/VO	$\rightarrow \infty$	Atmosphere without TiO and VO opacities <i>during</i> the GCM calculations; no post-hoc additions or modifications.

6.2 Methods

6.2.1 Model atmospheres

General overview

In this work, we consider four different 3D models of the atmosphere of WASP-76b, based on outputs of the SPARC/MITgcm global circulation model (Showman et al. 2009). For the setup of the GCM simulations, we refer the reader to Parmentier et al. (2018) and Chapter 4. All models assume chemical equilibrium, such that the abundances in each atmospheric cell are only a function of metallicity, C/O ratio (both set to solar value), and the local pressure and temperature. In addition, the GCM accounts for condensation through “rainout”, whereby a certain fraction of a species (e.g., Fe or Mg) is removed from a cell when the local temperature lies below the (pressure-dependent) condensation temperature of a condensate containing that species (e.g., Visscher et al. 2010). The process is called rainout, because it assumes that condensates instantly settle to a deeper layer where they do not impact the radiation balance of the atmosphere.

The four models are summarised in Table 6.1. Our nominal model is the same as the weak-drag model from Chapter 4. It has a drag timescale $\tau_{\text{drag}} = 10^5$ s, which has been found to provide a better match to the WASP-76b observations than a drag-free atmosphere (Chapter 4; May et al. 2021; Savel et al. 2022; Gandhi et al. 2022). The drag timescale represents the typical time it takes for an air parcel to lose a significant fraction of its kinetic energy. It encapsulates a number of different processes, such as turbulent mixing (Li & Goodman 2010), Lorentz-force braking of winds of charged particles due to the planet’s magnetic field (Perna et al. 2010a), and Ohmic dissipation (Perna et al. 2010b). As a result of drag forces, the equatorial jet of the planet is suppressed, such that the atmospheric dynamics are dominated by the day-to-night flow.

The second model we consider is the cold-morning-limb model from Chapter 4 (see “modification 2” in Fig. 4.14), in which we artificially reduce the temperature of the leading limb. Consequently, the atmosphere features a strong thermal asymmetry between the (hotter) trailing limb and (cooler) leading limb. In Chapter 4, we demonstrated that this model is able to reproduce the shape of the iron signal of WASP-76b (Ehrenreich et al. 2020; Kesseli & Snellen 2021), as opposed to an atmosphere without an east-west asymmetry. In the cold-morning-limb model, the absorption lines undergo an increasing blueshift during the first half of the transit, but they retain a constant Doppler shift of about -8 km/s during

the second half.

Our third model is an optically-thick-clouds model à la [Savel et al. \(2022\)](#), who reported that the iron signal of WASP-76b can also result from an atmosphere with optically thick clouds. In one of their best-fitting models, they assume the presence of an optically thick cloud deck extending at most 10 scale heights (~ 4.3 dex in pressure) above the intersection between the local temperature profile and the Al_2O_3 condensation curve. The vertical extent of the cloud is less than 10 scale heights in case the temperature profile and the condensation curve intersect again at some lower pressure. We add an optically thick cloud deck to our GCM output in exactly the same way (clouds are added post-hoc, so the temperature structure in the GCM is calculated *without* clouds). The rationale for selecting Al_2O_3 is that this is the cloud species with the highest condensation temperature. Hence, it will have the most drastic impact on the planet’s transmission spectrum, as it can exist in hotter regions compared to other cloud species. Because cloud physics is complicated (e.g., [Helling & Woitke 2006](#); [Gao & Benneke 2018](#); [Gao et al. 2018](#)), this modelling approach is very much a simplification of reality. However, the model forms a good *limiting case* – it allows to assess the strongest impact that clouds can possibly have on the CCF signal.

Our final model is the atmosphere without TiO and VO from Chapter 4. This represents a scenario in which TiO and VO are cold-trapped due to condensation ([Spiegel et al. 2009](#); [Parmentier et al. 2013](#); [Beatty et al. 2017](#)). To emulate the effects of cold-trapping, the opacities of TiO and VO are set to zero during the GCM calculations. Because these molecules are important short-wave absorbers, their absence will change both the dynamics and the temperature structure of the atmosphere. As shown in Chapter 4, the no-TiO/VO model naturally has a large temperature asymmetry between its trailing and leading limb, owing to a strong hotspot shift on the dayside that extends to relatively low pressures. Furthermore, our no-TiO/VO model is drag-free ($\tau_{\text{drag}} \rightarrow \infty$), so it features an equatorial jet. The model provides a good test to assess which observational features are robust against a variety of different modelling assumptions.

Mapping pressures onto altitudes

As described in Chapter 4, the GCM uses pressure as a vertical coordinate. However, to compute the transmission spectrum of the planet, the atmosphere must be defined on an altitude grid. Thus, before we can feed the models into the radiative-transfer framework, we need to perform the mapping $P \rightarrow z$ in every atmospheric column, with P the pressure and z the altitude coordinate. To this end, we follow the approach from Chapter 4 (see Section 4.3.2), whereby we assume that the atmosphere is an ideal gas in hydrostatic equilibrium. For every atmospheric cell i , we compute the scale height as follows:

$$H_i = \frac{k_B T_i}{\mu_i g_i}, \quad (6.1)$$

with k_B the Boltzmann constant, T_i the cell’s temperature, μ_i its mean-molecular weight, and g_i its gravity.

One important improvement we make compared to Chapter 4 is that we also account for mean-molecular weight variations across the atmosphere when computing H_i , in addition to temperature and gravity variations. On most of the dayside, the mean-molecular weight is significantly lower than on the nightside due to hydrogen (H_2) dissociation – lowering its value from $\mu \approx 2.33 m_{\text{H}}$ to $\mu \approx 1.27 m_{\text{H}}$ (with m_{H} the mass of a hydrogen atom). As a

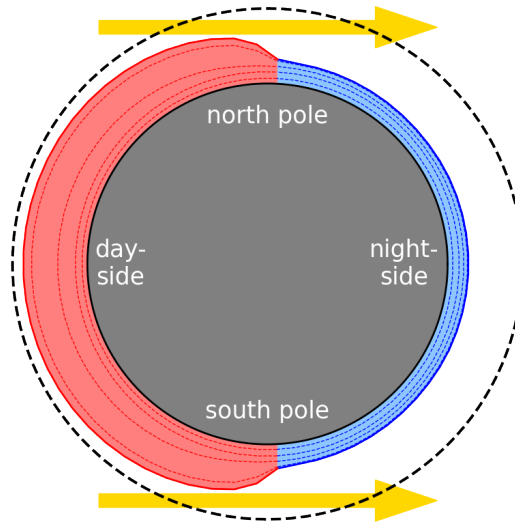


Figure 6.1: A cross-section of the nominal model of WASP-76b, with the interior (grey region), the dayside atmosphere (red region), and the nightside atmosphere (blue region) plotted to scale. The dayside is more “puffy” than the nightside due to its higher temperature and lower mean-molecular weight. Dashed lines indicate isobars with pressures 10^1 , 10^{-1} , 10^{-3} and 10^{-5} bar, respectively. The solid line marks the upper GCM boundary at $2 \mu\text{bar}$. When mapping the GCM output onto the altitude grid, we extrapolate the atmosphere to the same altitude everywhere (indicated by the black dashed circle). This means that the nightside extends to much lower (negligible) pressures than the dayside. Yellow arrows indicate light rays pointing towards the observer.

result, the scale-height difference between the dayside and the nightside of the models is even larger than suggested in Chapter 4. We verified, however, that (not) accounting for thermal dissociation in the $P \rightarrow z$ mapping does not drastically alter the shape of the final CCF signals (see Fig. 6.2), so the results from Chapter 4 remain valid.

Fig. 6.1 shows a *to-scale* plot of the nominal model mapped onto its altitude grid. The bottom of the atmosphere, with $P = 200$ bar and $g = 7.6$ m/s, is situated at a radius $R = 1.85 R_{\text{jup}}$. At the substellar point (on the dayside), the $10\text{-}\mu\text{bar}$ isobar lies at $R = 2.44 R_{\text{jup}}$. At the antistellar point (on the nightside), it lies at $R = 2.06 R_{\text{jup}}$. To prevent absorption lines from being “truncated” by the model boundaries in the radiative transfer, we extrapolate the entire atmosphere to a radius $R = 2.64 R_{\text{jup}}$ (black dashes in Fig. 6.1), assuming that temperatures, abundances, and wind speeds remain constant above the upper GCM boundary of $2 \mu\text{bar}$. Because the nightside has a much smaller scale height, it is extrapolated to trivially low pressures where the absorption is zero.

6.2.2 Radiative transfer

Monte-Carlo radiative transfer with gCMCRT

To compute transmission spectra associated with the 3D model atmospheres, we use gCMCRT (Lee et al. 2022b). In Chapter 4, we had to restrict our simulations to $\sim 10,000$ wavelength points for computational reasons, but with gCMCRT we can efficiently model high-resolution spectra across the full bandwidth of instruments like VLT/ESPRESSO and Gemini-S/IGRINS.

For each of the four WASP-76b models, we simulate the orbit over an angle of 31.3° degrees, covering the transit as well as ingress and egress. We compute 25 transmission spectra, equidistant in orbital phase. Furthermore, we assume an edge-on orbit, a semi-major axis of 0.033 AU , a stellar radius of $1.73 R_{\text{sun}}$, and an orbital period of 1.81 days – commensurate with the parameters of the WASP-76 system (West et al. 2016). We ignore effects of limb darkening as these were reported have a negligible impact on the Doppler shifts obtained from cross-correlation (Savel et al. 2022).

As in Chapter 4, we also compute spectra associated with individual sectors on the limb (see Fig. 2.2 in Chapter 2): the trailing equator, the trailing pole(s), the leading pole(s), and the leading equator. The trailing (*leading*) equator is the limb region between -45° and $+45^\circ$ latitude that is last (*first*) to appear in front of the star during ingress. The trailing (*leading*) poles are the regions between -90° and -45° , and $+45^\circ$ and $+90^\circ$ that are last (*first*) to appear in front of the star during ingress. All sectors span a quarter of the limb, but as shown in Fig. 2.2 in Chapter 2, the poles are disjoint. For a tidally locked planet, the trailing regions rotate towards the observer, while the leading regions rotate towards the star (away from the observer).

Modelling spectra in the optical (Fe and TiO signals)

In the optical, we model the transit of the four WASP-76b models across the full ESPRESSO wavelength range ($0.38\text{--}0.79 \mu\text{m}$) at a spectral resolution $R = 300,000$ (three times the ESPRESSO resolution). This results in a total of $\sim 220,000$ wavelength points. For memory-related reasons, we split the computation in two batches of $\sim 110,000$ wavelength points and we stitch the spectra together at the end. Since we read all opacity data at once at the start of the simulation, the GPU memory needs to hold the full 3D opacity structure of the atmosphere at *each* wavelength.

In the radiative transfer, we include (continuum) opacities associated with H_2 , He, and H scattering, collision-induced absorption (CIA) by $\text{H}_2\text{--H}_2$ and $\text{H}_2\text{--He}$, and bound-free and free-free transitions of H^- . References to these opacities can be found in Table 2 in Lee et al. (2022a). Also, we consider the following line species: Fe, Fe II, K, Na, Ti, Mn, Mg, Cr, Ca II, TiO, VO, H_2O , and OH. Atomic opacities are taken from the Kurucz & Bell (1995) database and we apply pressure broadening using a code based on Kurucz & Avrett (1981). In Chapter 4, the atomic opacities were generated with HELIOS-K (Grimm et al. 2021) and no pressure broadening was applied. Furthermore, HELIOS-K imposed a line-wing cut-off, as opposed to our current treatment. The opacities of TiO and VO are from the EXOPLINES database (Gharib-Nezhad et al. 2021a), and were generated by Gharib-Nezhad et al. (2021b) using the TOTO (McKemmish et al. 2019) and the VOMYT (McKemmish et al. 2016) line lists. For H_2O , we use the POKAZATEL line list (Polyansky et al. 2018). Finally, the OH opacities are taken from HITEMP (Rothman et al. 2010).

Compared to Chapter 4, we thus make a total of four changes to the radiative transfer. Firstly, we use iron line lists with pressure broadening and no line-wing cut-off, and we use opacities for a larger number of species. Secondly, we account for variations in mean-molecular weight when evaluating the scale height (see Section 6.2.1). Thirdly, we reduce the spectral resolution from 500,000 to 300,000. Finally, we consider the full ESPRESSO wavelength range instead of a small set of $\sim 10,000$ wavelength points. Fig. 6.2 depicts the effect that each of these changes has on the iron signal of the cold-morning-limb model originally presented in Chapter 4. The figure shows that the “new” iron opacities and the

new resolution do not significantly impact the CCF map. As expected, the new scale heights and the new wavelength range cause some changes, but the overall trends in the CCF map remain the same.

Modelling spectra in the infrared (CO, H₂O, and OH signals)

In the infrared, we model the transit of the four WASP-76b models across the full IGRINS wavelength range (1.42–2.42 μm) at $R = 135,000$ (three times the IGRINS resolution). This leads to $\sim 71,000$ wavelength points. We can afford a lower resolution here as the absorption features of the relevant molecules tend to be intrinsically broader than in the optical, so they can still be resolved at a lower resolution. We performed a comparison similar to Fig. 6.2 to verify that the Doppler shifts obtained from cross-correlation remain the same (within 0.5 km/s) at higher spectral resolutions.

To compute the infrared spectra, we consider the same continuum opacities as in the optical. Additionally, we use the line species CO (Li et al. 2015), H₂O (Polyansky et al. 2018), OH (Rothman et al. 2010), CH₄ (Hargreaves et al. 2020), CO₂ (Rothman et al. 2010), HCN (Barber et al. 2014), and NH₃ (Coles et al. 2019).

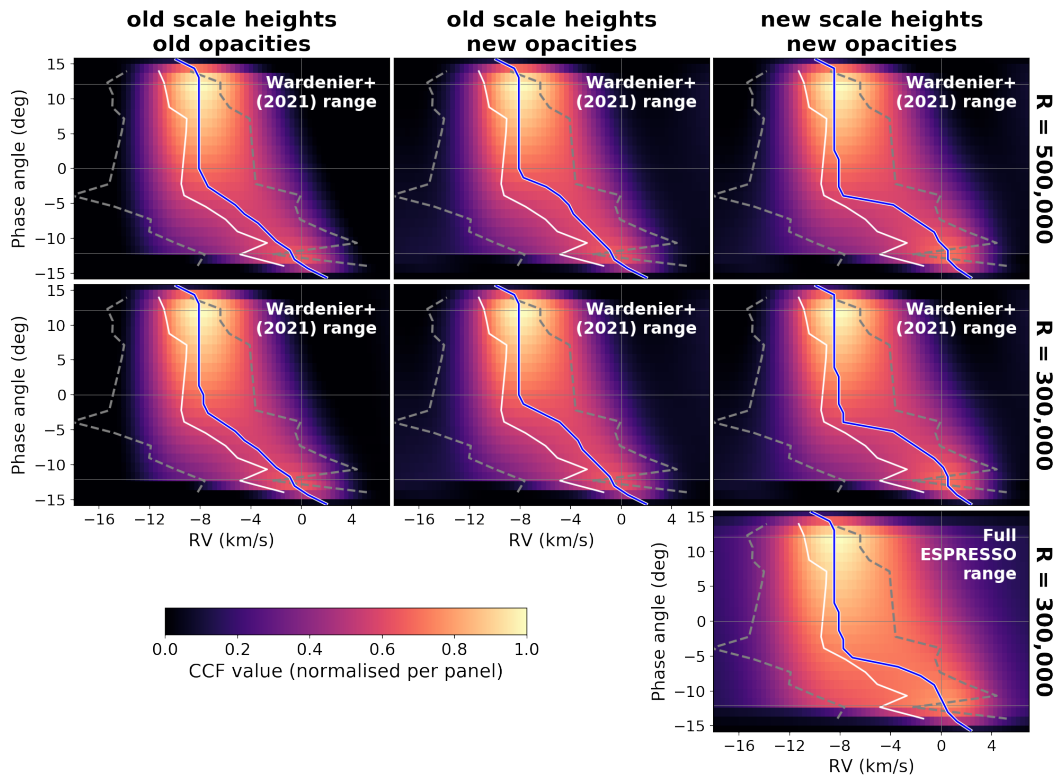


Figure 6.2: CCF maps for iron (Fe or Fe I) in the cold-morning-limb model. The panel in the top left shows the CCF map as presented in Chapter 4, while the panel in the bottom right shows the CCF map computed for *the same atmosphere* in this work. The other panels illustrate how the CCF map is impacted by each of the four “modelling changes” discussed in Section 6.2.2. In each panel, the blue curve indicates the maximum value of the CCF at each orbital phase. The white curve is the iron signal of WASP-76b observed by Ehrenreich et al. (2020). Grey dashes indicate the FWHM of this signal.

6.2.3 Computing observables

CCF maps

For each transit, we cross-correlate all 25 spectra with a template (see Section 2.2.1 in Chapter 2 for relevant equations). This gives rise to a CCF map with Doppler shift (radial velocity) as a horizontal coordinate and orbital phase as a vertical coordinate. We compute CCF maps for Fe and TiO (based on the optical spectra), as well as for CO, H₂O, and OH (based on the infrared spectra). To generate the template for a species X , we compute the mid-transit spectrum of the nominal model *without* Doppler shifts, whereby we only include the opacities of the continuum and X . Before we perform the cross-correlation, we subtract the continuum from both the templates and the spectra. We do this by splitting a spectrum into bins of 1000 wavelength points and fitting a low-order polynomial to the minima of these bins. We then subtract the polynomial from the spectrum to obtain a “flat” baseline. This procedure mimics the steps taken in the analysis of real high-resolution data.

We also compute CCF maps associated with the four limb sectors. As demonstrated in Chapter 2, the CCF map of the full limb can be interpreted as the sum of the CCF maps of the individual sectors, thanks to the linearity of the cross-correlation. The benefit of this approach is that it allows to link certain features of the CCF map to specific atmospheric regions.

K_p – V_{sys} maps

In most high-resolution datasets, the CCF values associated with individual integrations must be “stacked” across the whole transit to get a strong enough planet detection. A common way to do this is by constructing a K_p – V_{sys} map (e.g., Chapter 4; Brogi et al. 2012). The signal emerging in the K_p – V_{sys} map can be seen as a time average, because it is a sum over all orbital phases.

Once the CCF map of a certain species is computed, we obtain the corresponding K_p – V_{sys} map by integrating the CCF values along a curve of the form

$$v(\phi) = V_{\text{sys}} + K_p \sin(\phi), \quad (6.2)$$

with $v(\phi)$ the radial velocity at phase angle $\phi \in [-15.7^\circ, +15.7^\circ]$, V_{sys} the systemic velocity, and K_p the orbital velocity. In other words:

$$\text{SNR}(K_p, V_{\text{sys}}) = \frac{1}{\sigma} \sum_i^{N_\phi} \text{CCF}(\phi_i, v(\phi_i)). \quad (6.3)$$

In this equation, SNR is the value of the K_p – V_{sys} map at (K_p, V_{sys}) , σ is a scaling factor, and N_ϕ the number of simulated transit spectra. For each orbital phase, we obtain the CCF value at $v(\phi_i)$ by linearly interpolating between the two values at the nearest radial velocities in the CCF map.

6.2.4 Computing absorption regions

Following the approach from Chapter 5, we also compute absorption regions for each of the atmospheric models (see Section 5.3.2). The information needed to infer these regions is a byproduct of the radiative transfer.

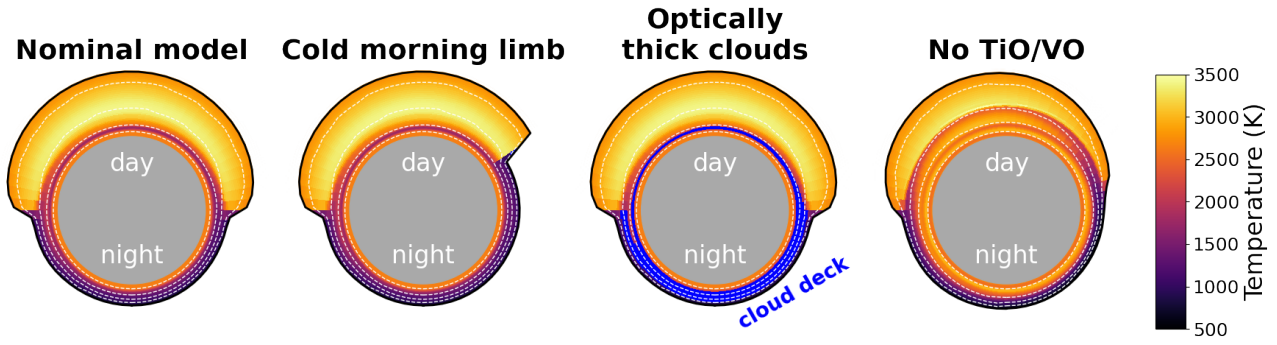


Figure 6.3: The temperature in the equatorial plane of the four models considered in this work (see Table 6.1). Note that the relative size of the atmosphere has been exaggerated for visualisation purposes – see Fig. 6.1 for the correct scale. White dashes indicate isobars with pressures 10^1 , 10^{-1} , 10^{-3} and 10^{-5} bar, respectively. The solid black line marks the upper GCM boundary at $2 \mu\text{bar}$. The dark blue patch in the optically-thick-clouds model shows the extent of the Al_2O_3 clouds, which are modelled according to the description in Savel et al. (2022).

The idea is that the spectrum does not contain any information about parts of the atmosphere where all the light is absorbed ($e^{-\tau} \sim 0$) or where all the light is transmitted ($e^{-\tau} \sim 1$). Instead, the observation probes the region where the *transition* from optically thick to optically thin occurs. Hence, given a wavelength λ , we define the absorption region as being spanned by all transit chords that satisfy $\beta < e^{-\tau} < 1 - \beta$. In Chapter 5, we opted for $\beta = 0.1$ and $\beta = 0.01$, and we named the corresponding regions the 10–90% and the 1–99% absorption regions, respectively.

The condition $\beta < e^{-\tau} < 1 - \beta$ only constrains the extent of the absorption regions in the altitude direction. However, to obtain a region that is finite *along* the line of sight as well, we only select the central part of the transit chords where the total optical depth increases from $\beta\tau$ to $(1 - \beta)\tau^1$. These two conditions allow us to infer the approximate regions that are probed by the transmission spectrum at a certain wavelength. Because we “truncate” the transit chords along the line of sight, the extent of the absorption regions is also independent of the (arbitrary) upper model boundary.

6.3 Results & discussion

6.3.1 3D temperatures, abundances, and line-of-sight velocities

Fig. 6.3 shows the temperature structure of the four WASP-76b models from Table 6.1 in the equatorial plane. As discussed in Section 6.2.1, the daysides are more “puffy” than the nightsides, owing to their higher temperature and lower mean molecular weight. The daysides also feature a strong thermal inversion. For example, at the substellar point in the nominal model, the temperature increases from ~ 1700 K at 1 bar to ~ 3500 K at 1 mbar. The nightside does not feature a thermal inversion and this is the reason why the cloud deck mostly spans 10 scale heights in the optically-thick-clouds scenario. At the antistellar point, the temperature drops from ~ 1700 K at 1 bar to ~ 1000 K at $10 \mu\text{bar}$.

¹As motivated in Chapter 5, this definition ensures that an absorption region is symmetric about the limb plane in the limit of a uniform 1D atmosphere.

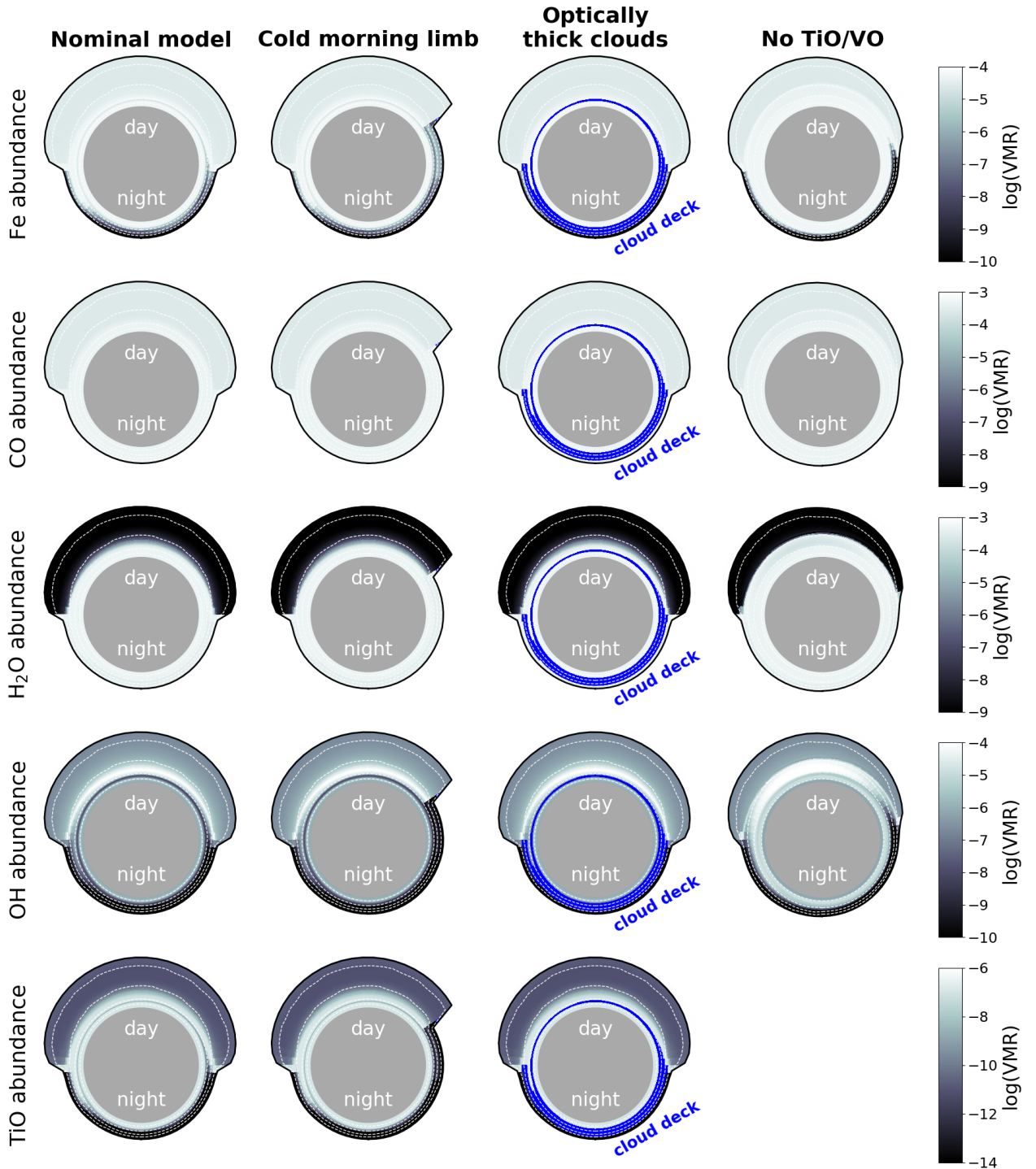


Figure 6.4: The abundances of Fe, CO, H₂O, OH, and TiO (one species per row) in the equatorial plane of the four models considered in this work (see Table 6.1). Note that the relative size of the atmosphere has been exaggerated for visualisation purposes. White dashes indicate isobars with pressures 10^1 , 10^{-1} , 10^{-3} and 10^{-5} bar, respectively (the planet's transmission spectrum probes pressures below 10^{-1} bar). The solid black line marks the upper GCM boundary at $2 \mu\text{bar}$. The dark blue patch in the optically-thick-clouds model shows the extent of the Al_2O_3 clouds, which are modelled according to the description in Savel et al. (2022).

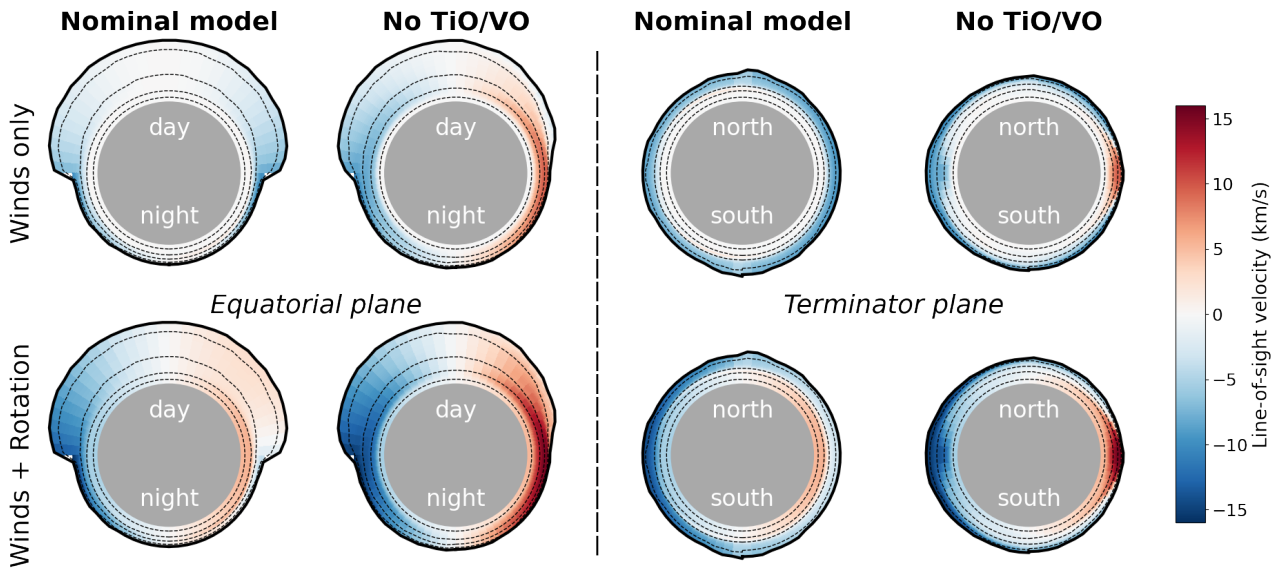


Figure 6.5: Line-of-sight velocities of the nominal model and the no-TiO/VO model at mid-transit, in the equatorial plane (left half of the figure) and the terminator plane (right half). The top row shows the line-of-sight velocities due to *winds only*, while the bottom row shows the line-of-sight velocities that result from the combination of winds and planetary rotation. At the equator, the rotational velocity of WASP-76b is ~ 5.3 km/s. Black dashes indicate isobars with pressures 10^1 , 10^{-1} , 10^{-3} and 10^{-5} bar, respectively (the planet’s transmission spectrum probes pressures below 10^{-1} bar).

Fig. 6.4 shows the abundances of Fe, CO, H₂O, OH, and TiO across the equatorial plane. All species have a unique 3D spatial distribution. Iron is abundant on the dayside, but absent on the nightside due to condensation. Water, on the other hand, is abundant on the nightside, but subject to thermal dissociation on the dayside (Parmentier et al. 2018). These “mirrored” chemical distributions imply that iron lines mainly probe the dayside of the planet, while the water lines mainly probe the nightside.

The CO abundance is nearly constant across the atmosphere – its value does not vary by more than ~ 0.3 dex. Because CO has a strong triple bond between its constituent atoms, it is neither affected by condensation, nor by thermal dissociation. In fact, the only ultra-hot Jupiter hot enough to dissociate CO is KELT-9b (Kitzmann et al. 2018). Consequently, the absorption lines of CO are the most reliable gauge of the 3D temperature structure and wind profile of the planet. They only probe spatial variations in temperature and dynamics, and not so much in chemistry. See Savel et al. (2023) for further discussion.

The distribution of OH is a bit more complicated. On the dayside, the molecule forms when water is dissociated into OH and atomic hydrogen. However, higher up in the atmosphere, OH itself also falls prey to thermal dissociation, producing atomic oxygen and atomic hydrogen. As a result, the OH abundance first increases with altitude and then decreases. On the nightside, OH is absent, because hydrogen and oxygen are contained in water at lower temperatures.

Finally, TiO is subject to both dissociation on the dayside and condensation on the nightside. Therefore, the only observable TiO is present in a narrow region around the limb where the temperature is *lower* than the dissociation temperature, but *higher* than the condensation temperature of TiO.

Fig. 6.5 shows the line-of-sight velocities v_{LOS} due to winds (and planetary rotation) in

the equatorial plane and the terminator plane of the nominal and the no-TiO/VO model, at mid-transit. These are the velocities by which the opacities in different cells are Doppler-shifted during the radiative transfer. $v_{\text{LOS}} < 0$ implies that absorbers are moving towards the observer, causing a blueshift to the transmission spectrum, while $v_{\text{LOS}} > 0$ means that absorbers are moving away, inducing a redshift. As illustrated in Fig. 6.5, the nominal model only features day-to-night winds (both planes are completely blueshifted in the top row), such that the only redshift contributions come from rotation (see bottom row). The no-TiO/VO model has an equatorial jet and this is why half of the *equatorial* plane is blueshifted, while the other half is redshifted. Note, though, that the jet only occupies a small region in the *terminator* plane, spanning an angle of ~ 25 degrees at pressures $\lesssim 1$ bar on both limbs (the latitudinal extent of the jet is of the order of the equatorial Rossby deformation radius – see Showman & Polvani 2011). However, despite the smaller “effective area” occupied by superrotating winds compared to the day-to-night flow, it may still be possible to make inferences about the equatorial jet based on the absorption signal of the full limb (e.g., Loudén & Wheatley 2015).

6.3.2 CCF maps for the nominal model

Fig. 6.6 depicts the CCF maps of the four limb sectors and the full limb of the *nominal model*, for all species. The CCF maps of the individual sectors can be seen as the “building blocks” of the more complicated absorption signal that emerges from the entire atmosphere. This is because the CCF map of the full limb is the sum of the maps of the limb sectors. Figs. 6.7 and 6.9 show the absorption regions that are probed on the trailing part of the equatorial plane by (randomly chosen) line cores of Fe, CO, H₂O, OH, and TiO, respectively.

Recap: two important effects

In Chapter 4 (see Fig. 4.11), we showed that there are two important effects that drive the Doppler shift of iron in the nominal model: (i) the variation in the signal strengths of the limb sectors during the transit, and (ii) atmospheric dynamics. In tandem, these effects cause the absorption signal to become *increasingly* blueshifted during the transit, even though there is *no* significant thermal or chemical asymmetry between the planet’s trailing and the leading limbs. On top of this “baseline behaviour”, limb asymmetries (e.g., Savel et al. 2023) can further enhance changes in the Doppler shift over time (see Section 6.3.3).

Effect (i) is due to the day-night temperature contrast of the planet, in combination with tidally-locked rotation. Ignoring the contribution from winds, the absorption signal of the redshifted leading limb becomes *weaker* during the transit, as the dayside rotates out of view. On the other hand, the signal of the blueshifted trailing limb becomes *stronger*, as the dayside rotates into view. Therefore, in a scenario without winds, the absorption signal of the full limb transitions from being mainly redshifted in the first half of the transit to being mainly blueshifted in the second half².

Effect (ii), atmospheric dynamics, impacts the absorption signal of the planet in multiple ways. Firstly, winds shift the whole CCF to negative radial velocities, as the day-to-night flow causes the whole terminator plane to be blueshifted (see Fig. 6.5). Secondly, they “smoothen” the CCF map, resulting in a more gradual change of the net Doppler shift

²See the third row of Fig. 4.11 in Chapter 4 (nominal model w/o winds).

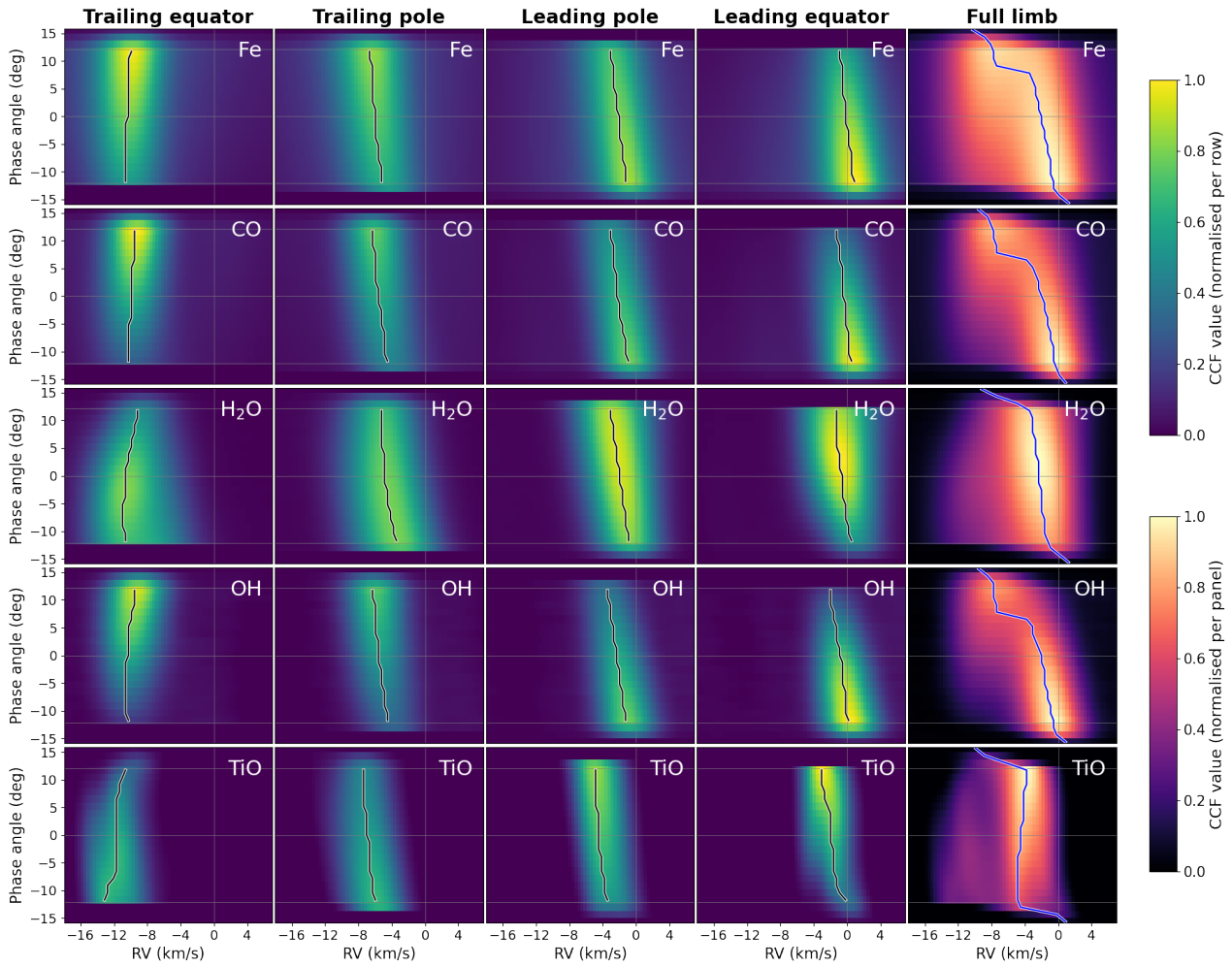


Figure 6.6: CCF maps for each of the limb sectors of the nominal model (first four columns), for each of the species considered in this work (rows). The right column contains the CCF maps of the full limb. For each species, the CCF maps of the limb sectors are normalised to the overall maximum of the four maps. The CCF maps of the full limb are normalised to their own maximum.

as a function of orbital phase. Finally, the angle between the polar wind vectors and the line-of-sight vector becomes smaller during the transit (see Fig. 4.12 in Chapter 4). This projection effect causes the absorption signals associated with the polar sectors to become more blueshifted over time. The signal of the leading equator shows the same behaviour.

Fe signals

The first row of Fig. 6.6 shows the CCF maps for iron. As mentioned in the previous paragraph, the iron signals of the nominal model were already presented in Chapter 4, but not for the entire ESPRESSO wavelength range. Although the atmosphere does not feature strong limb asymmetries, the iron lines become progressively more blueshifted during the transit, owing to effects (i) and (ii).

In Chapter 4 (see Section 4.5.1) we suggested that the change in signal strength of the limb sectors was because the observation first probes the nightside on the trailing limb, and later the dayside – with the exact opposite occurring on the leading limb. However, Fig.

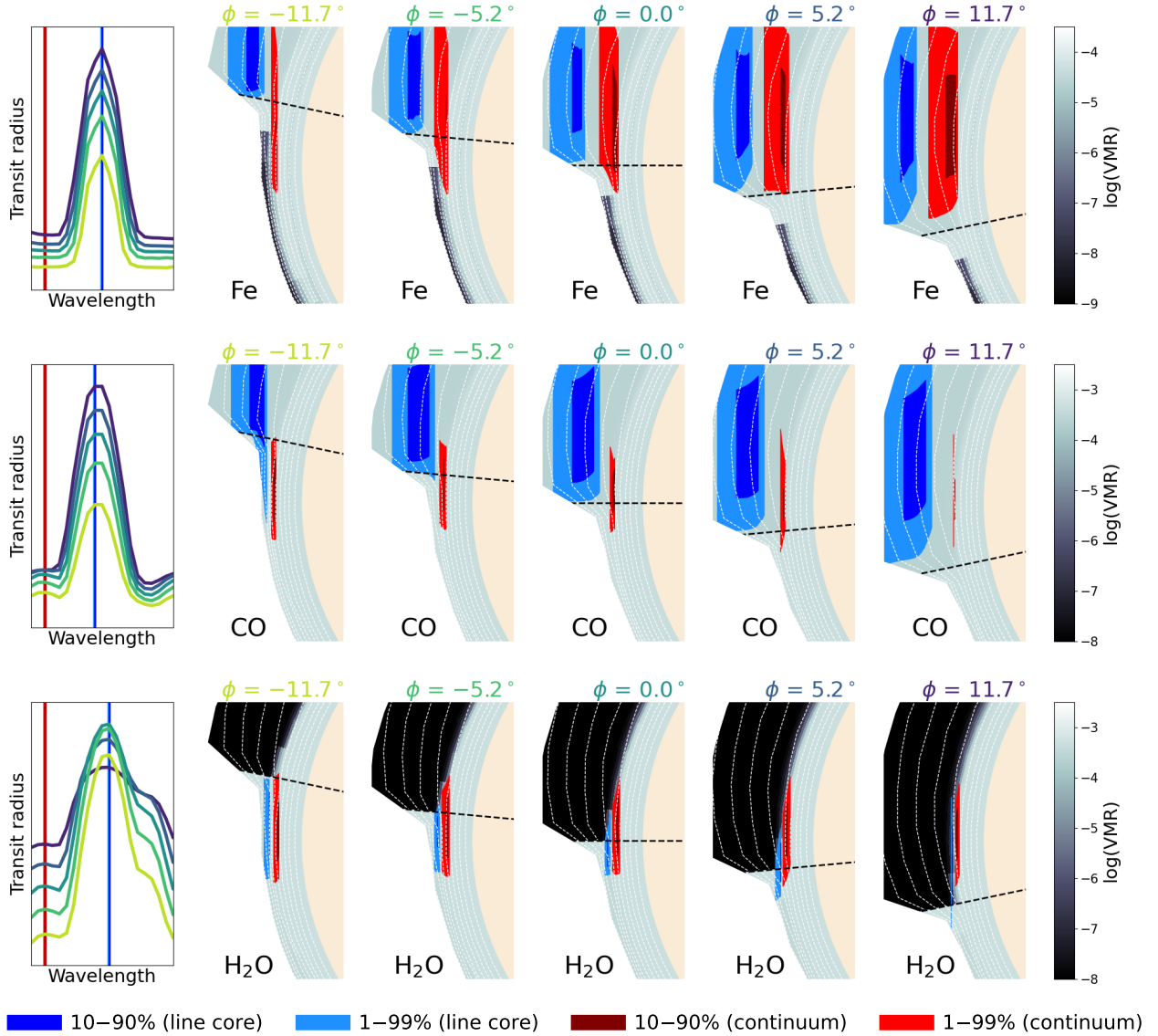


Figure 6.7: Absorption regions in the trailing part of the equatorial plane of the nominal model, for Fe (top row), CO (middle row), and H₂O (bottom row). For all species, absorption regions are plotted at two wavelengths, one inside a line core (blue) and one in the continuum (red). The 10–90% and 1–99% absorption regions are visualised at five different orbital phase angles ranging from -11.7° (just after ingress) to $+11.7^\circ$ degrees (just before egress). In each panel, the colourmap depicts the abundance of the relevant species, while the black dashed line marks the terminator plane. The dayside lies "above" this line and the nightside lies "below" this line. Furthermore, the white dashes indicate isobars that go down from 10 to 10^{-7} bar, in steps of 1 dex. The left panels show the absorption lines of the trailing equator at the five orbital phases (note that these only contribute for 25% towards the full spectrum).

6.7 demonstrates that something else is going on. Inside an iron line core, the absorption region lies on the dayside *at every orbital phase*. The reason why the signal of the trailing limb becomes stronger, though, is the fact that the projected separation (onto the limb plane) between the absorption region of the line core (in blue) and the absorption region of the continuum (in red) becomes larger during the transit. As shown in the top-left panel of Fig. 6.7, this causes an iron line to become stronger relative to its continuum, which is exactly what the magnitude of the CCF encodes. Therefore, in the case of iron, changes to a sector's signal strength are a consequence of geometry, rather than absorption regions shifting between the dayside and the nightside of the planet. However, the day-night contrast is still crucial for the projection effect to occur.

Furthermore, Fig. 6.7 illustrates that if iron was uniformly distributed across the atmosphere, its absorption lines would still only probe the dayside (see also the next paragraph about CO). Hence, it is *not* the 3D chemical map of iron that confines its absorption regions to the dayside. Instead, the scale-height difference between the dayside and the nightside causes a “shielding effect” – because the dayside is more puffy, the absorption lines probe altitudes at which the opacity of the nightside is negligible.

CO signals

The second row of Fig. 6.6 shows the CCF maps of CO. Both the CCF maps and the absorption regions of CO (see Fig. 6.7) display nearly identical behaviour compared to iron. Although the abundance of CO is uniform across the atmosphere, its absorption lines virtually only probe the dayside. That is, the 10–90% absorption regions of the CO line core are situated on the dayside at all orbital phases. The reason for this is the “shielding effect” discussed in the previous paragraph. Stellar light rays first encounter the dayside, and the $\tau \sim 1$ region lies at altitudes where the nightside does not contribute to the total optical depth.

For CO, the signal strength of the trailing equator also increases during the transit, again due to a projection effect. Around the CO line plotted in Fig. 6.9, the “continuum” is caused by water absorption. As a result, the absorption region of the continuum behaves exactly like that of water in Fig. 6.7 (see also the next paragraph). Interestingly, at $\phi = -11.7^\circ$ the CO line core and its adjacent continuum probe *different* sides of the planet.

H₂O signals

The third row of Fig. 6.6 shows the CCF maps of water. Remarkably, the phase-dependence of the signal strengths displays the opposite behaviour compared to iron and CO. For iron and CO, the trailing-equator signal becomes *stronger* during the transit, but for water it becomes *weaker*. The absorption regions in Fig. 6.7 demonstrate why this is the case. At the start of the transit, a water line core probes the nightside. Then, as the planet rotates, its absorption region shifts towards the dayside. However, because of the lack of water at low pressures (due to thermal dissociation), the absorption region is “pushed” down to higher pressures on the dayside. At these higher pressures, the absorption regions of the line core and the continuum lie closer together, which explains why the signal strength of the trailing limb decreases over the transit. Naturally, the opposite occurs on the leading limb, as shown by the CCF maps of the limb sectors in Fig. 6.6.

Based on the behaviour of the individual limb sectors, one would expect the blueshift of the full limb to *decrease* during the transit. After all, the signal strength of the (least

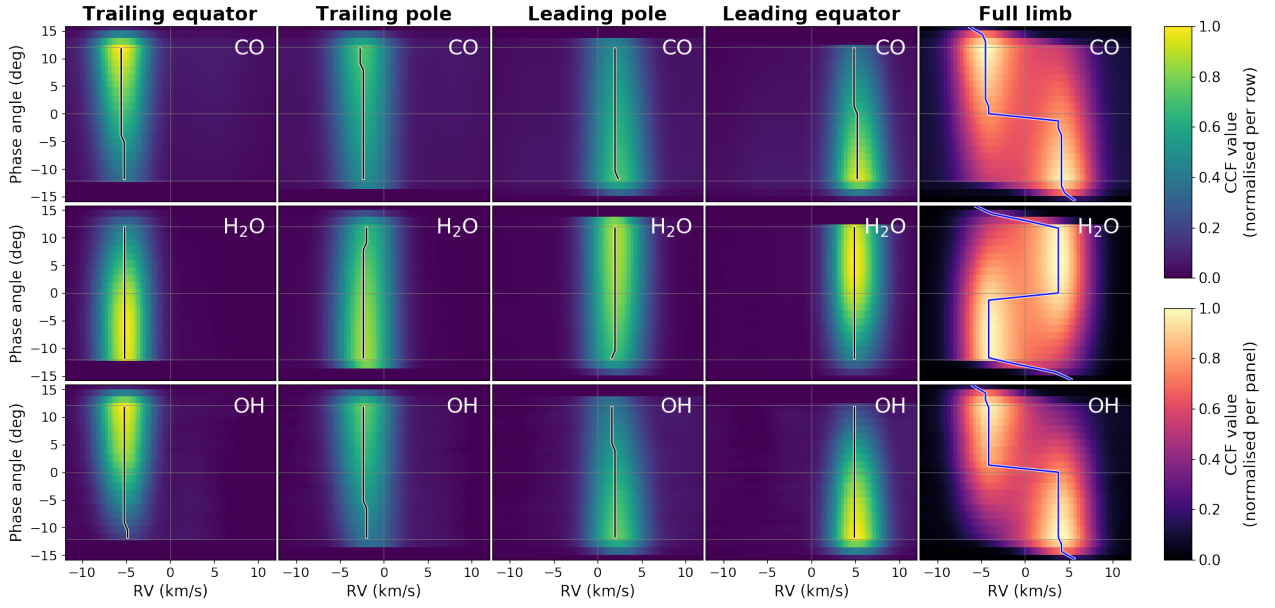


Figure 6.8: CCF maps for CO, H₂O, and OH in the nominal model when only considering Doppler shifts due to rotation (and not due to winds). During the transit, the signal strengths of the trailing sectors *increase* in the case of CO and OH, but they *decrease* in the case of H₂O. The leading sectors show the opposite behaviour. For each species, the CCF maps of the limb sectors are normalised to the overall maximum of the four maps. The CCF maps of the full limb are normalised to their own maximum.

blueshifted) leading sectors becomes stronger over time. However, the reason why the net Doppler shift of the planet does *not* decrease is that the signals of the leading limb are stronger than those of the trailing limb over almost the entire transit. Therefore, the water signal of the full limb is dominated by the leading sectors, which are subject to an *increasing* blueshift over time.

In Fig. 6.8 we show the CCF maps for CO, H₂O, and OH when *only* Doppler shifts due to planet rotation are taken into account (with winds set to zero). In this case, the water signal of the full limb does exhibit a decreasing blueshift, because the signal of the trailing limb is stronger than that of the leading limb in the first half of the transit. Hence, it is the wind profile that causes the trailing-limb signals in Fig. 6.6 to be weaker than the leading-limb signals. On the trailing limb, the variance in probed wind speeds is larger, causing the line contrast to become smaller and the CCF of the trailing sectors to become broader. Ultimately, this causes the water signal to look relatively similar to that of iron and CO, even though the water lines probe completely different regions of the atmosphere. Our result is in qualitative agreement with Savel et al. (2023) and Beltz et al. (2023), who also found an increasing blueshift for water based on their 3D models of WASP-76b.

The absorption regions of water become very narrow towards the end of the transit ($\phi = 11.7^\circ$ in Fig. 6.7). This is because the distance between isobars is smaller at higher pressures. Also, the absorption regions coincide with a steep vertical gradient in the water abundance. Therefore, shifting the transit chord to a lower pressure will result in a sharp decrease in integrated abundance (and thus optical depth), while moving it to higher pressures will result in $\tau \gg 1$.

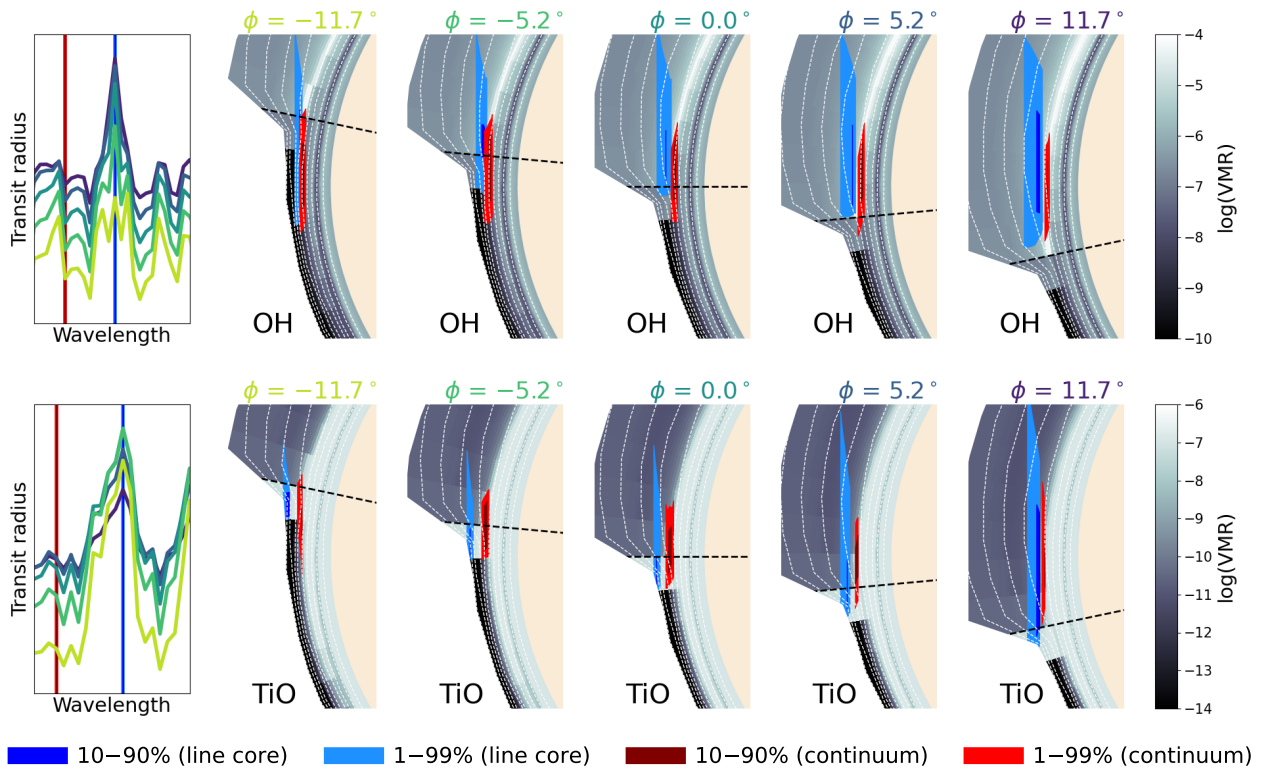


Figure 6.9: Same as Fig. 6.7, but for OH (top row) and TiO (bottom row).

OH signals

The fourth row of Fig. 6.6 shows the CCF maps of OH. In the nominal model, the OH signal resembles that of iron and CO. However, the strength of the OH signal drops by a factor ~ 2 during the transit. Also, Fig. 6.6 demonstrates that the change in the signal strength of the trailing equator (as well as the other limb sectors) is more extreme than for the other species – at the start of the transit it is almost zero. Fig. 6.9 illustrates the cause of this significant variation. Because the nightside is depleted of OH and because the higher altitudes on the dayside have a low OH abundance, the absorption regions of the line core and the continuum overlap at the start of the transit. This produces a negligible CCF signal. However, as the planet rotates, the more OH-abundant parts of the dayside rotate into view, and the line contrast increases.

TiO signals

The bottom row of Fig. 6.6 shows the CCF maps of TiO. Whereas the other species clearly show an increasing blueshift during the transit, the blueshift of TiO is *decreasing* in the nominal model (albeit marginally). The reason for this is that the signal strengths of the limb sectors behave like those of water (see Fig. 6.6). Yet, in contrast to water, the signal of the trailing sectors is strong enough at the beginning to contribute to the Doppler shift of the full limb. At the end of the transit, the CCF map is dominated by the signal from the leading sectors.

As shown in the figures, the signal of the (most blueshifted) trailing limb becomes *weaker*

during the transit, as the absorption region of the TiO line core shifts from the nightside to the dayside. We note, though, that the absorption region very much hinges on the TiO abundances in the first column on the nightside (see Fig. 6.9), where the temperature profile allows for TiO to exist at all pressures. Without this column, the absorption regions would have been situated at lower altitudes, resulting in much weaker absorption lines (the column *has* to exist, though, as the atmosphere transitions from dayside to nightside). On the other hand, if the temperature gradient at the terminator was smoother, for example due to H₂ dissociation/recombination (Bell & Cowan 2018; Komacek & Tan 2018; Tan & Komacek 2019; Roth et al. 2021), TiO would have existed across a wider range of longitudes. Therefore, in this model, it is the steepness of the temperature gradient at the terminator that determines whether or not TiO may be observable.

6.3.3 CCF maps for other models

Fig. 6.10 shows the CCF maps computed for all models and all species (only the CCF maps of the full limb are shown). The colourmaps were normalised per species to allow for inter-model comparisons. Because TiO is cold-trapped in the no-TiO/VO model, it is not observable. Hence, there are 19 maps in total, rather than 20.

Fe signals

As expected, the cold-morning-limb model in Fig. 6.10 shows a strong increase in blueshift over the first half of the transit. The reason for this is that the signals of the leading sectors are much weaker compared to the nominal model (see Fig. 4.15 in Chapter 4). Hence, the signals of the trailing sectors already start to dominate the sum before mid-transit. After mid-transit, the blueshift remains constant, because the only contributions to the signal come from the trailing sectors. For further discussion, we refer to Chapter 4.

The CCF map of the optically-thick-clouds model is very similar to that of the nominal model, suggesting that adding a cloud deck has minimal impact on the iron signal. The reason for this is that the absorption regions of iron on the dayside lie at much *higher* altitudes compared to the optically thick clouds on the nightside (see Figs. 6.4 and 6.7). Yet, the signal strength of the full limb does decrease slightly as a result of clouds. This is because the cloud deck lies at higher altitudes than the absorption regions of the continuum in the cloud-free atmosphere. Since the cloud deck is nearly symmetric, the signals of the trailing and leading limbs are affected equally – the line contrast and the magnitude of the CCF become marginally smaller, but the shape does not change. Thus – in this particular model – we find that nightside clouds are unable to mute the iron absorption signal, as it originates from too high altitudes. To make a cloud mute the absorption features of a species, as in Savel et al. (2022), it should be located at a significantly higher altitude than the continuum in the cloud-free case. Based on our modelling efforts, we still find that a temperature (or scale-height) asymmetry between the morning and the evening limb is the most likely explanation for the strongly blueshifted iron signals of WASP-76b (Ehrenreich et al. 2020; Kesseli & Snellen 2021) and WASP-121b (Borsa et al. 2021). Further comparisons need to be carried out to elucidate any differences between our models and those of Savel et al. (2022).

The iron signal of the no-TiO/VO model also exhibits stronger blueshifts compared to the nominal model. This is also related to a temperature asymmetry (see Fig. 6.3). Due to a large hotspot shift on the dayside, the 3D temperature structure of the model is lopsided,

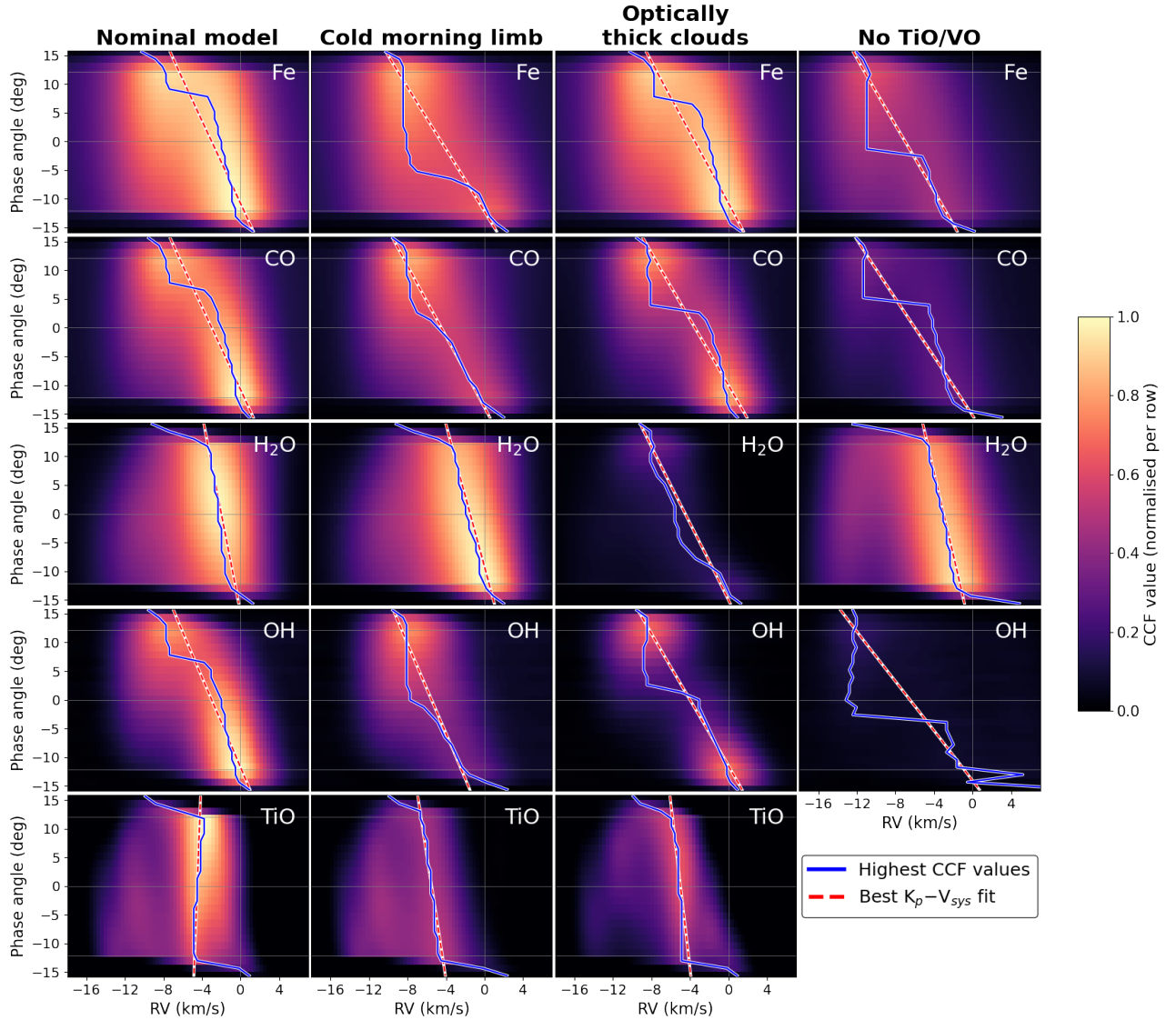


Figure 6.10: CCF maps of Fe, H₂O, CO, OH, and TiO (one species species per row) for each of the four models considered in this work (see Table 6.1 and Figs. 6.3–6.5). All maps were normalised to their own maximum. The colourmap shows the value of the cross-correlation as a function of orbital phase (vertical axis) and velocity shift between the template and the transmission spectrum of the planet (horizontal axis). The blue curve in each panel indicates the maximum value of the CCF at each orbital phase. The red dashed line corresponds to the K_p and V_{sys} values that give rise to the maximum SNR values in the K_p - V_{sys} map.

with the trailing limb being hotter and more extended than the leading limb. Hence, the signal of the blueshifted trailing limb contributes more strongly to the CCF map of the full planet.

CO signals

The behaviour of CO across the different models is very similar to that of iron (e.g., compare the first and the second rows in Figs. 6.6 and 6.10). In the cold-morning-limb model, for example, the signal also undergoes a strong increase in blueshift during the first half of the

transit, owing to the temperature asymmetry between the trailing and the leading sectors.

The CCF map of CO is somewhat affected by the presence of optically thick clouds. This indicates that there are weaker CO lines that probe the atmosphere at *lower* altitudes, and which are thus muted by the cloud deck. For these weaker lines, the absorption regions are likely to lie partly on the dayside and partly the nightside, as CO is equally abundant on both hemispheres. With this in mind, the (stronger) CO line considered in Fig. 6.9 may not be fully representative. However, note that the blue absorption regions plotted in Fig. 6.9 only pertain to the line *core* – the line wings, which also contribute to the CCF, must probe lower altitudes.

H₂O signals

The signals of the nominal model, the cold-morning-limb model, and the no-TiO/VO model show the same behaviour, with the no-TiO/VO signal being slightly more blueshifted due to stronger day-to-night winds. The reason for this is that the 3D spatial distribution of water in each of the models is very similar. Water is present on the nightside, as well as at higher pressures on the dayside where the scale heights on the trailing limb and the leading limb are still the same (see Fig. 6.4). Consequently, the temperature asymmetries in the cold-morning-limb model and the no-TiO/VO model do not manifest in the CCF maps.

In contrast to iron, the presence of optically thick clouds strongly suppresses the water signal. This is because the cloud deck is situated at roughly the same altitude as the water absorption regions. Hence, the line contrast is small and the vast majority of water lines are muted.

OH signals

The OH signal of the cold-morning-limb model also features an increasing blueshift during the first half of the transit. However, the signal from the leading sectors is very weak. The reason for this is that the colder leading limb is depleted of OH, while the high-altitude part of the dayside that is in view does not have sufficient OH abundance to cause significant absorption. In the second half of the transit, the trailing sectors completely dominate the absorption signal. The same idea holds for the no-TiO/VO model, which does not have any detectable OH on the leading limb.

Just like water, OH probes relatively low altitudes. Therefore, the introduction of optically thick clouds heavily mutes the OH absorption lines. At mid-transit, the absorption signal is almost zero. The strongest contributions come from the leading equator around ingress and from the trailing equator around egress. Again, however, it is questionable whether optically thick clouds allow for OH to be detected at all, given that the CCF signal only emerges from a narrow range of orbital phase angles.

TiO signals

In the cold-morning-limb model, the contribution from the leading equator is zero (not shown in a plot). This is why the TiO signal is more blueshifted than in the nominal model. Additionally, the TiO signal appears to have a more bimodal structure. As a result, the signal is “smeared” over a range of K_p and V_{sys} values (see Fig. 6.11), which could make TiO harder to detect in this scenario. When optically thick clouds are introduced, TiO absorption

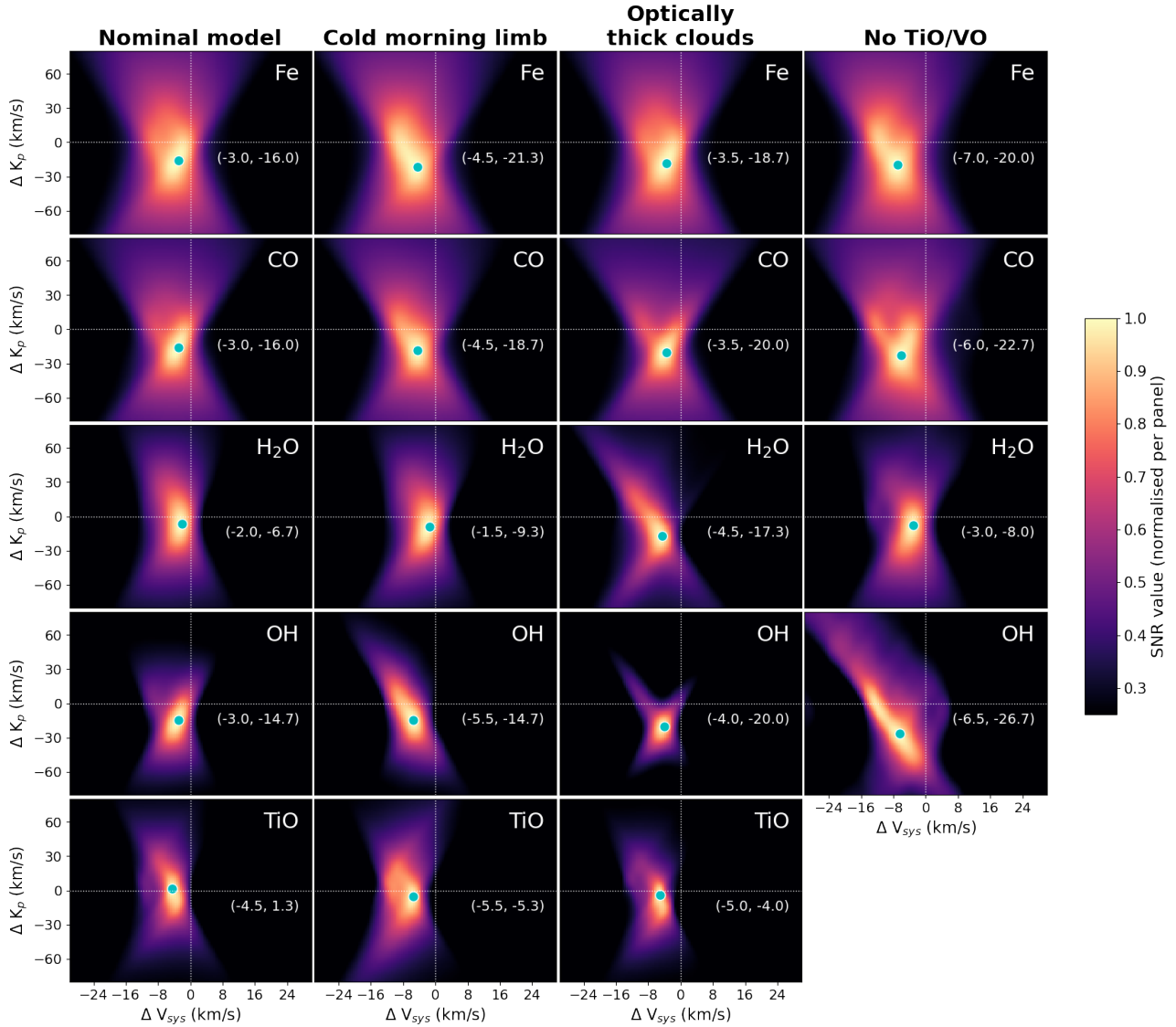


Figure 6.11: K_p – V_{sys} maps of Fe, CO, H_2O , OH, and TiO (one species species per row) for each of the four models considered in this work (see Table 6.1 and Figs. 6.3–6.5). All maps were normalised to their own maximum. The colourmap shows the value of the SNR (signal-to-noise ratio), as a function of orbital velocity (vertical axis) and systemic velocity (horizontal axis) *relative to the planetary rest frame*. The blue dot in each panel indicates the maximum SNR value.

is muted in all limb sectors except the leading pole (not shown). This is why the blueshift of the full-limb signal in Fig. 6.10 closely resembles that of the leading pole in Fig. 6.6.

6.3.4 K_p – V_{sys} maps

Systematic peak offsets

Fig. 6.11 shows the K_p – V_{sys} maps associated with the CCF maps from Fig. 6.10. Because the absorption signals all exhibit Doppler shifts in the planetary rest frame, the SNR peaks in the K_p – V_{sys} maps are offset from (0,0) km/s. All SNR peaks, except for the TiO signal of the nominal model, are consistently located at *lower* V_{sys} and *lower* K_p values than would

be expected based on the orbital motion of the planet and the radial velocity of the star. The red dashed curves in Fig. 6.10 illustrate why this is the case. These are the curves that give rise to the highest integrated SNR value (equation 6.3). Because all absorption signals are blueshifted on average, the best-fitting curve has a negative horizontal offset, yielding $\Delta V_{\text{sys}} < 0$. Also, because the signals become *more* blueshifted over time (with the exception of TiO in the nominal model), the slope of the curve is negative, corresponding to $\Delta K_p < 0$.

Along the V_{sys} axis, the offset of the SNR peak is typically a few km/s. To zeroth order, ΔV_{sys} can be interpreted as the average wind speed across the terminator. The maximum shift we encounter is $\Delta V_{\text{sys}} = -7$ km/s for the iron signal of the no-TiO/VO model. Intuitively, it makes sense that the shifts are the largest for this model, as it has no drag and thus the highest wind speeds.

Along the K_p axis, the peak offset can be more significant. Typically, the K_p shift is much larger than the Doppler shift measured from the CCF at any orbital phase. This is because the K_p value does not necessarily encode information about the absolute value of the Doppler shift. Rather, it reflects the *rate of change* of the Doppler shift of the full limb during the transit (and thus how steep the slope of the best fitting K_p - V_{sys} needs to be). For this reason, signals with a strong phase-dependence (such as iron in the cold-morning-limb model and CO in the no-TiO/VO model) show the most extreme values of ΔK_p .

Estimating the K_p shift of a planet

For species that mainly probe the dayside (e.g., Fe, CO, and OH) of the atmosphere, we can make a zeroth-order estimation of ΔK_p . To this end, we assume that the absorption signal is dominated by the leading limb (equatorial and polar sectors) at the start of the transit and by the trailing limb (equatorial and polar sectors) at the end of the transit. The average rotational velocity $\bar{v}$ of a limb is given by

$$\bar{v} = \pm 2 \frac{v_{\text{eq}}}{\pi}, \quad (6.4)$$

with v_{eq} the rotational velocity of the planet at the equator. This expression is the average value of $\pm v_{\text{eq}} \cos(\theta)$ over the domain $\theta \in [-\pi/2, +\pi/2]$. Furthermore, during transit it holds that $\sin(\phi) \approx \phi$, such that the difference in radial velocity ΔRV between two orbital phases is

$$\Delta RV = 2\pi K_p \left(\frac{\Delta\phi}{360^\circ} \right), \quad (6.5)$$

with $\Delta\phi$ the difference in orbital phase angle. In the planetary *rest frame*, $\Delta RV = 2\bar{v}$ between the start and the end of the transit. This change in radial velocity will translate to an offset ΔK_p , which can be calculated as follows:

$$\Delta K_p = \frac{\Delta RV}{2\pi} \left(\frac{360^\circ}{\Delta\phi} \right) = \frac{2v_{\text{eq}}}{\pi^2} \left(\frac{360^\circ}{\Delta\phi} \right) = \frac{4R_p}{\pi P} \left(\frac{360^\circ}{\Delta\phi} \right), \quad (6.6)$$

with R_p and P the radius and the orbital period of the planet, respectively. For WASP-76b, $v_{\text{eq}} \approx 5.3$ km/s. Furthermore, if we take $\Delta\phi \approx 24^\circ$, we find that $\Delta K_p \approx 16$ km/s³. This value

³ $\Delta\phi \approx 24^\circ$ is the difference in phase angle between the second and the third contact of the transit (during which the entire planet is in front of the star). We assume that the contributions from ingress and egress are small compared to the integrated CCF signal between these two points.

is in good agreement with the K_p shifts in Fig. 6.10.

Comparison to observations

A considerable number of HRS observations of ultra-hot Jupiters have revealed peak offsets that could hint at atmospheric dynamics and/or 3D spatial variations in temperature and chemistry (e.g., Gibson et al. 2020; Borsa et al. 2021; Landman et al. 2021; Merritt et al. 2021; Rainer et al. 2021; Kesseli et al. 2022; Maguire et al. 2022; Prinoth et al. 2022; Sánchez-López et al. 2022). In what follows, we will specifically focus on results obtained for WASP-76b.

Kesseli et al. (2022) conducted a spectral survey of WASP-76b using the ESPRESSO dataset from Ehrenreich et al. (2020). For most of the species detected in the dataset, they found negative K_p and/or V_{sys} offsets, which is in general agreement with this work. Note, though, that some of these species (such as Na and Ca II) probe the atmosphere at pressures that are lower than our GCM boundary of 2 μbar , which could explain some of the discrepancies between the models and the data.

In the infrared, CARMENES observations of WASP-76b revealed positive K_p offsets for H_2O (+50 km/s, Sánchez-López et al. 2022) and OH (+35 km/s, Landman et al. 2021), suggesting a *decreasing* blueshift of the absorption lines over the course of the transit. Based on our current modelling efforts, any large positive offset in K_p is hard to explain, especially for species that probe the dayside of the atmosphere. Further modelling studies will be required to interpret these observations.

6.4 Conclusion

Developing a deeper understanding of the “3D-ness” of exoplanet atmospheres is crucial to fully leverage the information content of both their high-resolution and low-resolution spectra. With JWST delivering its first data (e.g., The JWST Transiting Exoplanet Community Early Release Science Team et al. 2022) and a new generation of ground-based telescopes (E-ELT, GMT, TMT) on the horizon, modelling studies that bridge the gap between theory and observation play an essential role in the interpretation of current and future observations. In this work, we simulated the cross-correlation signals of Fe, CO, H_2O , OH, and TiO for four different 3D models of a benchmark ultra-hot Jupiter (WASP-76b) in transmission. Because ultra-hot Jupiters show extreme spatial variations in temperature and chemistry across their terminators, their transmission spectra contain a wealth of information about the 3D structure of the atmosphere. We summarise our most important findings below:

- Different species have different 3D spatial distributions across the atmospheres of ultra-hot Jupiters. Hence, their absorption lines probe distinct regions of the limb. During the transit, a single line can probe the planet’s dayside and nightside at different orbital phases, respectively.
- For species that probe the dayside of an ultra-hot Jupiter, the net blueshift should *increase* during the transit, even in the absence of an east-west asymmetry (e.g., due to a hotspot offset). The increasing blueshift is caused by the day-night contrast of the planet, in combination with tidally locked rotation. Species that probe the dayside are refractories and alkali metals, as well as molecules like CO and OH.

- Thermochemical asymmetries between the planet’s trailing and leading limb can *enhance* changes in Doppler shift during the transit.
- For species that probe the nightside, the blueshift can *either* increase or decrease during the transit, depending on the relative strengths of the absorption signals associated with the trailing and the leading limb. In our nominal model, we found an increasing blueshift for H₂O, but a decreasing blueshift for TiO.
- All our CCF maps show a net blueshift ($\Delta V_{\text{sys}} < 0$), while all our CCF maps except one show an *increasing* blueshift during the transit ($\Delta K_p < 0$). In K_p – V_{sys} space, this translates to a negative offset from the expected peak position along both the K_p and the V_{sys} axis. V_{sys} offsets are typically a few km/s, while K_p offsets can be as big as -20 km/s. If observed for ultra-hot Jupiters, such offsets can be attributed to 3D effects in the atmosphere.
- To account for the fact that different species probe different regions of the atmosphere, 1D retrievals in high resolution should retrieve *separate* temperature profiles and (ΔK_p , ΔV_{sys}) values for each species.

We now present some conclusions related to specific models and species considered in this study:

- Even though CO is uniformly distributed across the atmosphere of an ultra-hot Jupiter, it predominantly probes the dayside. This is because of a “shielding effect” – since the dayside is more extended than the nightside, CO absorption happens at high altitudes on the dayside where the nightside contribution to the optical depth is zero.
- In our nominal model, the water signal becomes increasingly blueshifted during the transit, *in spite* of the phase-dependence of the signal strengths of the individual limb sectors. A larger variance in probed wind speeds on the trailing limb causes the CCF signal of the trailing limb to be weaker compared to the leading limb. Hence, the water signal is shaped by a “wind asymmetry”.
- The thermal asymmetry in the cold-morning-limb model further enhances the blueshifts of iron, CO, and OH. This is because the absorption signal from the leading limb quickly subsides, such that the CCF map becomes dominated by contributions from the (most blueshifted) trailing limb. The simulated absorption signals of Fe, CO, and OH show the same trend as the iron signal of WASP-76b observed by [Ehrenreich et al. \(2020\)](#) – see also Chapter 4.
- Water absorption lines are strongly muted by optically thick clouds in our model. This is because the cloud deck is situated at the same altitudes as the absorption regions of water. Conversely, the iron absorption signal is not significantly affected by clouds, as iron probes higher altitudes on the dayside that reach above our cloud deck.
- At lower pressures, the only observable TiO is present around the terminator, in regions cooler than the dissociation temperature of TiO but hotter than its condensa-

tion temperature. Hence, the observability of TiO (if not already cold-trapped) will very much depend on the temperature gradient between the dayside and the nightside.

- To differentiate between the models considered in this study, one needs to measure the CCF signals of at least *two* species – for example iron and water.

Bibliography

- Barber R. J., Strange J. K., Hill C., Polyansky O. L., Mellau G. C., Yurchenko S. N., Tennyson J., 2014, *MNRAS*, **437**, 1828
- Beatty T. G., Madhusudhan N., Tsias A., Zhao M., Gilliland R. L., Knutson H. A., Shporer A., Wright J. T., 2017, *AJ*, **154**, 158
- Bell T. J., Cowan N. B., 2018, *ApJ*, **857**, L20
- Beltz H., Rauscher E., Kempton E., Malsky I., Savel A., 2023, *arXiv e-prints*, p. [arXiv:2302.13969](https://arxiv.org/abs/2302.13969)
- Borsa F., et al., 2021, *A&A*, **645**, A24
- Brogi M., Snellen I. A., De Kok R. J., Albrecht S., Birkby J., De Mooij E. J., 2012, *Nature*, **486**, 502
- Coles P. A., Yurchenko S. N., Tennyson J., 2019, *MNRAS*, **490**, 4638
- Dorn R. J., et al., 2023, *arXiv e-prints*, p. [arXiv:2301.08048](https://arxiv.org/abs/2301.08048)
- Ehrenreich D., et al., 2020, *Nature*, pp 1–7
- Gandhi S., Kesseli A., Snellen I., Brogi M., Wardenier J. P., Parmentier V., Welbanks L., Savel A. B., 2022, *MNRAS*, **515**, 749
- Gao P., Benneke B., 2018, *ApJ*, **863**, 165
- Gao P., Marley M. S., Ackerman A. S., 2018, *ApJ*, **855**, 86
- Gharib-Nezhad E., Iyer A. R., Line M. R., Freedman R. S., Marley M. S., Batalha N. E., 2021a, EXOPLINES: Molecular Absorption Cross-Section Database for Brown Dwarf and Giant Exoplanet Atmospheres, [doi:10.5281/zenodo.4458189](https://doi.org/10.5281/zenodo.4458189), <https://doi.org/10.5281/zenodo.4458189>
- Gharib-Nezhad E., Iyer A. R., Line M. R., Freedman R. S., Marley M. S., Batalha N. E., 2021b, *ApJS*, **254**, 34
- Gibson N. P., et al., 2020, *MNRAS*, **493**, 2215
- Grimm S. L., et al., 2021, *ApJS*, **253**, 30
- Hargreaves R. J., Gordon I. E., Rey M., Nikitin A. V., Tyuterev V. G., Kochanov R. V., Rothman L. S., 2020, *ApJS*, **247**, 55
- Helling C., Woitke P., 2006, *A&A*, **455**, 325
- Holmberg M., Madhusudhan N., 2022, *AJ*, **164**, 79
- Kesseli A. Y., Snellen I. A. G., 2021, *ApJ*, **908**, L17
- Kesseli A. Y., Snellen I. A. G., Casasayas-Barris N., Mollière P., Sánchez-López A., 2022, *AJ*, **163**, 107
- Kitzmann D., et al., 2018, *ApJ*, **863**, 183
- Komacek T. D., Tan X., 2018, *Research Notes of the AAS*, **2**, 36
- Kurucz R. L., Avrett E. H., 1981, *SAO Special Report*, 391
- Kurucz R., Bell B., 1995, *Atomic Line Data (R.L. Kurucz and B. Bell) Kurucz CD-ROM No. 23*. Cambridge, 23
- Landman R., Sánchez-López A., Mollière P., Kesseli A. Y., Louca A. J., Snellen I. A. G., 2021, *A&A*, **656**, A119
- Lee E. K. H., Prinoth B., Kitzmann D., Tsai S.-M., Hoeijmakers J., Borsato N. W., Heng K., 2022a, *MNRAS*, **517**, 240
- Lee E. K. H., et al., 2022b, *ApJ*, **929**, 180
- Li J., Goodman J., 2010, *ApJ*, **725**, 1146
- Li G., Gordon I. E., Rothman L. S., Tan Y., Hu S.-M., Kassi S., Campargue A., Medvedev E. S., 2015, *ApJSupplement Series*, **216**, 15
- Line M. R., et al., 2021, *Nature*, **598**, 580
- Louden T., Wheatley P. J., 2015, *ApJ*, **814**, 1
- Mace G., et al., 2018, in Evans C. J., Simard L., Takami H., eds, *Society of Photo-Optical Instrumentation Engineers (SPIE) Conference Series Vol. 10702, Ground-based and Airborne Instrumentation for Astronomy VII*. p. 107020Q, [doi:10.1117/12.2312345](https://doi.org/10.1117/12.2312345)
- Maguire C., Gibson N. P., Nugroho S. K., Ramkumar S., Fortune M., Merritt S. R., de Mooij E., 2022, *MNRAS*, **511**, 158
- May E. M., et al., 2021, *AJ*, **162**, 158
- McKemmish L. K., Yurchenko S. N., Tennyson J., 2016, *MNRAS*, **463**, 771

- Mckemmish L. K., Masseron T., Hoeijmakers H. J., Pérez-Mesa V., Grimm S. L., Yurchenko S. N., Tennyson J., 2019, [MNRAS](#), 488, 2836
- Merritt S. R., et al., 2021, [MNRAS](#), 506, 3853
- Parmentier V., Showman A. P., Lian Y., 2013, [A&A](#), 558, 91
- Parmentier V., et al., 2018, [A&A](#), 617
- Perna R., Menou K., Rauscher E., 2010a, [ApJ](#), 719, 1421
- Perna R., Menou K., Rauscher E., 2010b, [ApJ](#), 724, 313
- Polyansky O. L., Kyuberis A. A., Zobov N. F., Tennyson J., Yurchenko S. N., Lodi L., 2018, [MNRAS](#), 480, 2597
- Prinoth B., et al., 2022, [Nature Astronomy](#), 6, 449
- Rainer M., et al., 2021, [A&A](#), 649, A29
- Roth A., Drummond B., Hébrard E., Tremblin P., Goyal J., Mayne N., 2021, [MNRAS](#), 505, 4515
- Rothman L. S., et al., 2010, [J. Quant. Spectrosc. Radiative Transfer](#), 111, 2139
- Sánchez-López A., Landman R., Mollière P., Casasayas-Barris N., Kesseli A. Y., Snellen I. A. G., 2022, [A&A](#), 661, A78
- Savel A. B., et al., 2022, [ApJ](#), 926, 85
- Savel A. B., Kempton E. M. R., Rauscher E., Komacek T. D., Bean J. L., Malik M., Malsky I., 2023, arXiv e-prints, [p. arXiv:2301.01694](#)
- Showman A. P., Polvani L. M., 2011, [ApJ](#), 738, 71
- Showman A. P., Fortney J. J., Lian Y., Marley M. S., Freedman R. S., Knutson H. A., Charbonneau D., 2009, [ApJ](#), 699, 564
- Spiegel D. S., Silverio K., Burrows A., 2009, [ApJ](#), 699, 1487
- Tan X., Komacek T. D., 2019, [ApJ](#), 886, 26
- The JWST Transiting Exoplanet Community Early Release Science Team et al., 2022, arXiv e-prints, [p. arXiv:2208.11692](#)
- Visscher C., Lodders K., Fegley B., 2010, [ApJ](#), 716, 1060
- West R. G., et al., 2016, [A&A](#), 585, A126

Chapter 7

Summary & Outlook

7.1 Thesis summary

In this thesis, we explored the impact of the 3D atmospheric structure of ultra-hot Jupiters (UHJs) on their high-resolution transmission spectra. UHJs have a permanent dayside and a permanent nightside with vastly different temperatures and chemical compositions. Transmission spectra probe the terminator region of these planets, where the transition from the dayside to the nightside occurs. Getting a better handle on the “3D-ness” of exoplanets is important for constraining abundances in their atmospheres and understanding their formation and migration history. UHJs form excellent targets in this regard, as a lack of clouds provides observational access to their entire chemical inventory.

In **Chapter 2**, we introduced gCMCRT (see also [Lee et al. 2022](#)). gCMCRT is a Monte-Carlo radiative-transfer code that can compute phase-dependent transmission and emission spectra for any planet atmosphere. The code accounts for 3D variations in temperature, chemistry, and cloud coverage, as well as Doppler shifts caused by the planet’s rotation and 3D wind profile. In this thesis, we added high-resolution functionalities to gCMCRT, allowing the code to treat Doppler shifts induced by winds and rotation. We benchmarked the high-resolution mode against a 1D radiative-transfer code. Additionally, we showed that gCMCRT can produce transmission spectra for different limb sectors – these help to better understand how different parts of the atmosphere contribute to the planet’s overall absorption signal. Finally, we discussed singular-value decomposition (SVD), the cross-correlation function (CCF), and K_p - V_{sys} maps.

In **Chapter 3**, we reviewed high-resolution observations of 3D effects in UHJs. In general, these can be grouped into four categories: (i) phase-dependent Doppler shifts and peak offsets in K_p - V_{sys} maps, (ii) different Doppler shifts for different chemical species, (iii) phase-dependent signal strengths, and (iv) multi-peak features in K_p - V_{sys} maps. Additionally, we discussed previous modelling studies that simulated high-resolution spectra based on 3D global circulation models (GCMs).

In **Chapter 4** ([Wardenier et al. 2021](#)), we used gCMCRT to simulate transmission spectra of WASP-76b from outputs of the SPARC/MITgcm, focusing on the planet’s iron signal. We condensed the spectra into CCF and K_p - V_{sys} maps to study how “3D-ness” manifests in observations. We demonstrated that the signal strengths of different limb sectors change substantially with phase, due to the planet’s day-night contrast and tidally-locked rotation. Also, we showed that atmospheres with different drag timescales and with/without TiO and VO opacities give rise to different CCF signals. These result in peak offsets in the corresponding K_p - V_{sys} map. Finally, we demonstrated that an asymmetry between the trailing (evening) and leading (morning limb) is required to explain the observed iron signal for WASP-76b ([Ehrenreich et al. 2020](#)). This asymmetry could be a scale-height difference between both limbs, or condensation, which leads to the absence of iron on the leading limb.

In **Chapter 5** ([Wardenier et al. 2022](#)), we derived a new formula for the opening angle. In transmission spectroscopy, the opening angle of a planet quantifies how much “depth information” its spectrum contains (i.e., what swath of the atmosphere is probed along the line of sight). We used gCMCRT to compute the opening angle for a grid of planets with

different radii and equilibrium temperatures. We found that the opening angle is only a few degrees for planets cooler than ca. 500 K, while it can be as large as 25 degrees for (ultra-)hot Jupiters and 50 degrees for hot Neptunes. Finally, we showed that UHJs have an opening angle that is smaller than their rotation angle during the transit. This allows for time-resolved transmission spectroscopy observations that probe independent parts of the planetary limb during the first and second half of the transit.

In **Chapter 6** (Wardenier et al. 2023, submitted), we used gCMCRT to compute transmission spectra of WASP-76b across the entire wavelength range of VLT/ESPRESSO (optical) and GEMINI-S/IGRINS (infrared). We studied the absorption signals of Fe, TiO, CO, H₂O, and OH, which each have a different spatial distribution across the atmosphere. Based on our work, we concluded that the day-night contrast of ultra-hot Jupiters consistently leads to increasing blueshifts for species that probe the dayside (e.g., all refractories), even if they are distributed uniformly across the atmosphere, like CO. This should remain true in the absence of an east-west asymmetry on the planet, such as a hotspot shift. Species probing the nightside can be subject to either an increasing or a decreasing blueshift. Finally, we showed that our models yield systematic offsets in K_p - V_{sys} maps, whereby the K_p shift of a species can be much larger than its net Doppler shift at any orbital phase.

In **Appendix A** we present preliminary results of three transits observations of WASP-121b. We report significant detections of CO and H₂O, but not of OH.

7.2 Avenues for future research

In this section, we propose some ideas for future research that build on the material presented in this thesis.

7.2.1 Modelling emission spectra of ultra-hot Jupiters with gCMCRT

A logical next step would be to extend the work from Chapters 4 and 6 to emission spectroscopy. As described in Chapter 2, gCMCRT also has an emission mode that can be used to assess a wide range of 3D effects. Although multiple studies have already computed emission spectra from 3D GCM outputs (Zhang et al. 2017; Harada et al. 2021; Malsky et al. 2021; Beltz et al. 2021), there are still many questions that remain unanswered:

- What do the K_p - V_{sys} maps of different species look like at different orbital phases (pre-transit, post-eclipse, etc.)? How does the 3D structure of ultra-hot Jupiters translate to peak offsets in K_p - V_{sys} maps?
- How do the CCF signals of different disk sectors (analogous to limb sectors in transmission – see Fig. 2.2) behave as a function of orbital phase? What is the most insightful way to partition the planet disk into sectors?
- At a given orbital phase, what fraction of the flux is emerging from the dayside? To what extent does the dayside flux “contaminate” nightside spectra taken at pre-transit or post-transit? How could this affect inferences of nightside properties?
- How does the line contrast change as a function of orbital phase for different species?

- How is atmospheric dynamics (e.g., the presence of an equatorial jet) imprinted on high-resolution emission spectra?

Another avenue would be to study the role of clouds in emission, whose ability to (multiple) scatter photons can greatly affect the shape of the spectrum (e.g., [Taylor et al. 2021](#)). At high spectral resolution, multiple scattering is an especially rich problem, because a Doppler shift is imposed on a photon every time it scatters off a particle with a certain velocity. Because gCMCRT explicitly tracks the paths of individual photons, it forms the natural framework to account for multiple scattering.

7.2.2 Assessing 3D effects for a grid of hot gas giants

To systematically explore 3D effects across parameter space, gCMCRT could be used to post-process a grid of GCM outputs. Recently, [Roth et al. \(in prep.\)](#) computed an extensive grid of gas-giant atmospheres using the SPARC/MITgcm. Currently, the grid comprises six hundred¹ 3D atmospheric structures, spanning across 9 different equilibrium temperatures (ranging between 800 K to 2400 K), 3 metallicity values, 3 surface-gravity values, and 3 stellar masses/radii/temperatures. Furthermore, the grid includes models with/without magnetic drag, and with/without TiO and VO opacities. The goal of the study would be to identify where in parameter space 3D effects matter most, how they manifest in the observables, and which trends can be observed.

Figure 7.1 depicts a subset of 18 planets from the [Roth et al. \(in prep.\)](#) grid that were post-processed with gCMCRT ([Hood & Wardenier et al., in prep.](#)). Each planet in the figure has its own semi-major axis and rotation period, which are set by the stellar mass, the stellar temperature, and the equilibrium temperature of the planet (tidal locking is assumed for all planets in the grid). For each planet, we computed phase-dependent transmission spectra between 0.38 and 0.55 micron. The spectra were cross-correlated with a template of iron lines and subsequently turned in to a K_p - V_{sys} map.

Figure 7.1 shows clear trends for the K_p and V_{sys} offsets as a function of equilibrium temperature. Some curious behaviour occurs for the hottest planets (2200 K and 2400 K) around the smallest (and coolest) star. Because these planets have very short orbital periods, their rotation rates are so high that the trailing and leading limb become fully separated in wavelength space (due to opposite Doppler shifts). This results in two distinct peaks in the K_p - V_{sys} map with extreme values for ΔV_{sys} . The transit of the hottest planet covers one sixth of the entire orbit.

7.2.3 Preparing for the era of extremely large telescopes

Extremely large telescopes (ELTs), such as the GMT, the TMT and the E-ELT will revolutionise the field of high-resolution spectroscopy, as JWST is currently doing for low-resolution observations. In current high-resolution datasets, the planet signal is always buried in stellar/telluric noise (except for a few strong lines) and needs to be “teased out” using the cross-correlation technique. However, for the brightest star-planet systems (e.g., WASP-18b, WASP-76b, WASP-189b), spectrographs on ELTs will take observations in which the planet signal immediately stands out from the noise. This yields the prospect of assessing the shape/shift/strengths of thousands of individual lines (probing different pressures), rather

¹A. Roth, private communication

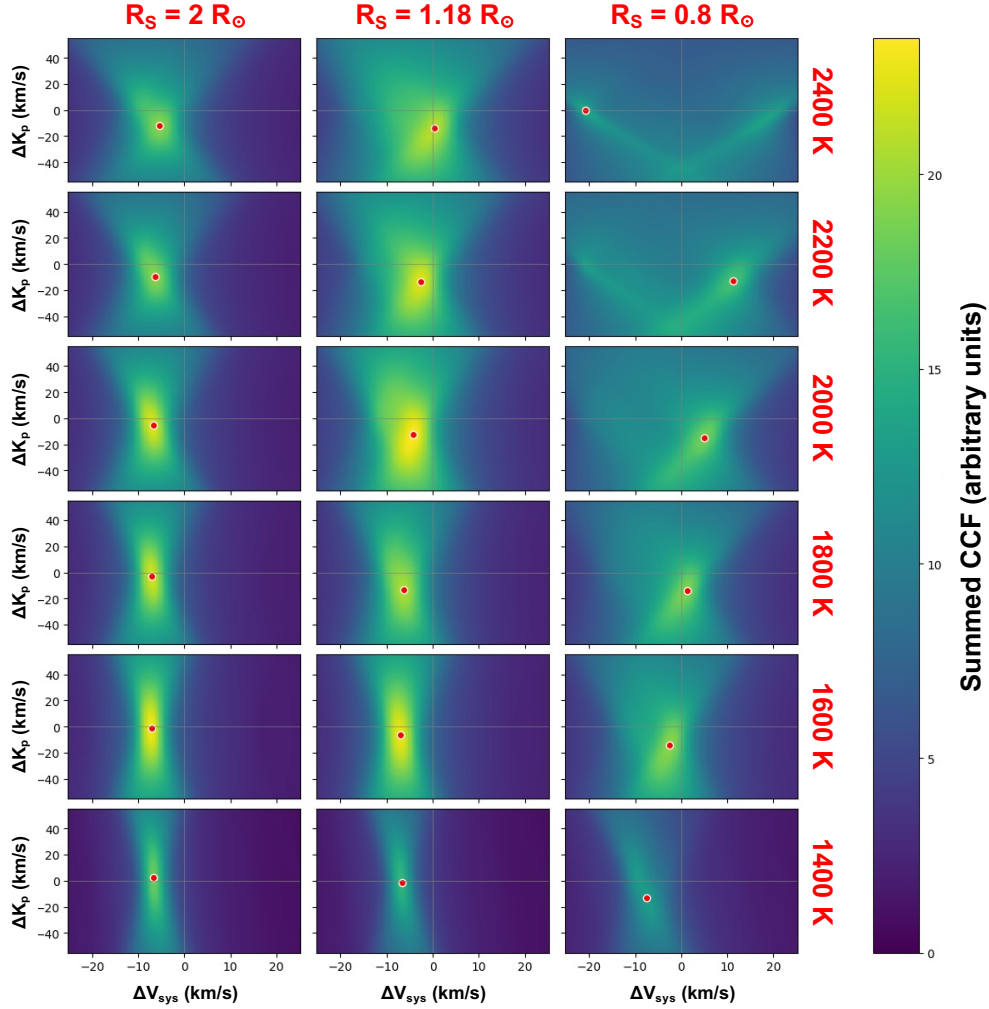


Figure 7.1: K_p - V_{sys} maps for iron (Fe I) based on the optical transmission spectra of 18 GCM outputs from the [Roth et al. \(in prep.\)](#) grid, post-processed with gCMCART. Each column represents a host star with a different radius R_s (and thus a different mass and effective stellar temperature), while each row represents a planet with a different equilibrium temperature T_{eq} . Each (R_s, T_{eq}) combination corresponds to a unique rotation period. Red markers indicate the maximum of each map. Image courtesy of T. Hood.

than relying on average quantities obtained from the cross-correlation. At the time of writing, no studies have been performed that realistically simulate transmission and emission observations of exoplanets with ELTs, and that evaluate the information content of the high signal-to-noise spectra they will produce.

An interesting project would be to combine gCMCART with an instrument simulation pipeline, such as `simMETIS`² (for E-ELT/METIS, [Brandl et al. 2018](#)), to produce realistic transmission and emission spectra for several benchmark exoplanets, ranging from ultra-hot Jupiters to Earth-analogues. The goal would be to demonstrate to the community what kind of science can be performed for what kind of planet, what the best observing strategies are, and what “3D information” can be inferred from the data. An example of this is constraining the wind speed on the trailing and leading limb of tidally locked planets based on their ingress and egress spectra (e.g., [Louden & Wheatley 2015](#)), or measuring the rotation rate

²See metis.strw.leidenuniv.nl/simmetis/

of cooler planets that are not synchronised. In addition, one could examine how well the Doppler shifts of individual spectral lines can be constrained, and how small/cold a planet must become for its “3D-ness” to no longer stand out from the noise, such that it can be well-fitted by a 1D spectrum. Such efforts are especially relevant for the characterisation of smaller planets around M dwarfs.

Bibliography

- Beltz H., Rauscher E., Brogi M., Kempton E. M. R., 2021, *AJ*, **161**, 1
- Brandl B. R., et al., 2018, in Evans C. J., Simard L., Takami H., eds, Vol. 10702, Ground-based and Airborne Instrumentation for Astronomy VII. SPIE, p. 107021U, doi:10.1117/12.2311492, <https://doi.org/10.1117/12.2311492>
- Ehrenreich D., et al., 2020, *Nature*, pp 1–7
- Harada C. K., Kempton E. M. R., Rauscher E., Roman M., Malsky I., Brinjikji M., DiTomaso V., 2021, *ApJ*, **909**, 85
- Lee E. K. H., et al., 2022, *ApJ*, **929**, 180
- Louden T., Wheatley P. J., 2015, *ApJ*, **814**, 1
- Malsky I., Rauscher E., Kempton E. M. R., Roman M., Long D., Harada C. K., 2021, *ApJ*, **923**, 62
- Taylor J., Parmentier V., Line M. R., Lee E. K. H., Irwin P. G. J., Aigrain S., 2021, *MNRAS*, **506**, 1309
- Wardenier J. P., Parmentier V., Lee E. K. H., Line M. R., Gharib-Nezhad E., 2021, *MNRAS*, **506**, 1258
- Wardenier J. P., Parmentier V., Lee E. K. H., 2022, *MNRAS*, **510**, 620
- Zhang J., Kempton E. M.-R., Rauscher E., 2017, *ApJ*, **851**, 84

Appendix A

A first look at three transits of WASP-121b observed with IGRINS

In this appendix, we present preliminary results of three transit observations of WASP-121b with Gemini-S/IGRINS (covering $1.42\text{--}2.42\ \mu\text{m}$ at $R = 45,000$), for which the author of this thesis was the PI. Because this is our first attempt at computing cross-correlations and $K_p\text{--}V_{\text{sys}}$ maps from the data, the results are by no means final yet. However, they do offer insight into the data quality, and the improvement of the planet signal when combining the three transits together.

A.1 Observations and data reduction

Observations

The data were taken on 25 February 2022 (00:28–04:32), 10 December 2022 (03:37–07:41), and 24 December 2022 (04:12–08:16). All dates and times are in UT. We followed the *typical IGRINS observing setup* as described on the IGRINS at Gemini webpage³, which uses an ABBA nodding pattern with an on-slit separation of $2.5''$. During each night, we observed about 30 minutes of stellar baseline before and after the transit, which itself lasts about 175 minutes. Including target acquisition and other overheads, this means that every observation lasted about 4 hours.

During transits 1 and 3, the exposure time was 100 seconds per frame (200 seconds per AB pair). For transit 2, the exposure time was 130 seconds (260 seconds per AB pair). The reason for this difference is not entirely clear. No notes were made of worse weather conditions in the observer log, and the signal-to-noise per frame is indeed higher for transit 2 than for transits 1 and 3. All in all, the higher exposure time for transit 2 is not an issue. 130 seconds is still well below the “Doppler-smearing” limit of the observation. This is the time it takes for the spectrum to shift by one resolution element on the detector ($\sim 6.7\text{ km/s}$ for IGRINS) due to the orbital motion of the planet.

Data reduction and cross-correlation

All datasets were pre-processed with the IGRINS pipeline package⁴ (PLP, Sim et al. 2014). We then conducted a wavelength-calibration⁵ as described in Section 2.3.1. Next, we performed an order-by-order singular value decomposition (SVD) to separate the planet signal from stellar and telluric contributions (see Section 2.3.2). For each IGRINS order, we removed the first 5 SVD components. This number is by no means optimised, and more work is required to investigate how the data-cleaning process impacts the final detection significances.

³sites.google.com/site/igrinsatgemini/proposing-and-observing

⁴PLP is publicly available from github.com/igrins/plp

⁵M. Line and M. Mansfield, private communication.

After the SVD, we performed a cross-correlation analysis (see Section 2.3.3) on the residual data, searching for the presence of CO, H₂O, and OH in the atmosphere of the planet. Template models were generated with gCMCRT, based on a GCM output of WASP-121b (Parmentier et al. 2018). For simplicity, we only calculated the transmission spectrum at mid-transit, ignoring any changes with orbital phase. To account for rotational broadening of the spectrum, we also included Doppler shifts due to planet rotation. Finally, before cross-correlating the templates with the data, we convoluted the templates with a Gaussian kernel to match the instrument resolution of 45,000.

K_p - V_{sys} maps were computed via the method described in Section 6.2.3. To convert (Σ CCF) values into SNR values, we divided the entire K_p - V_{sys} map by σ , with σ the standard deviation of the (Σ CCF) values in the region $V_{\text{sys}} < 0$. This is a region far away from the detection peak, and thus it should only contain noise⁶.

Combining the transits

We also made an attempt to combine the CCF and K_p - V_{sys} maps of the three transits together. For now, we just summed the CCF maps in the planet-rest frame, giving each transit an “equal weight” (i.e., not accounting for any differences in signal-to-noise between the observations). To this end, we interpolated every CCF map onto the same grid of RV and orbital-phase values, before performing the addition. There is no guarantee that this is the optimal way to proceed, and we plan to explore other methods in the future.

A.2 CCF and K_p - V_{sys} maps

Figs. A.1 and A.2 show the CCF maps for CO and water, respectively. In the left column, the planet signal manifests as a diagonal trail, because of orbital motion (K_p sets the slope of the trail and V_{sys} the offset). The right column shows the CCF maps in the planetary rest frame. As indicated in the maps, the total transit of WASP-121b spans ~ 34 degrees, including the ingress and egress phase.

Figs. A.3 and A.4 show the 1D CCFs for CO and water, respectively. These were obtained by summing the CCF maps along the phase axis in the planetary rest frame. Besides the CCF of the whole transit, we also plot the CCFs for the first and the second half of the transit, in order to explore differences in signal strength and Doppler shift.

Finally, Figs. A.5 – A.7 show the K_p - V_{sys} maps for CO, water, and OH, respectively. While we detect CO and water at high significance, we do not obtain a significant detection peak for OH.

CO signals

The plots in Figs. A.1 and A.3 show some considerable differences between the transits. In transit 1, the CO signal appears to be much stronger in the second half compared to the first half. In the other two transits, however, the CO signal is equally strong. This is also the result we obtain when adding the three CCF maps together. In transits 1 and 3, the CO signal appears to be subtly blueshifted, which is consistent with a day-to night flow on the

⁶Although this is a standard way to compute SNR values in high-resolution spectroscopy, it is problematic, because the values in a K_p - V_{sys} do generally not follow a normal distribution (due to correlated noise).

planet. The data also hint at small differences in Doppler shift between the first and the second half of the transit (especially in transit 3). Further analysis, such as Gaussian-peak fitting, should reveal whether these differences are significant.

Fig. A.5 shows the K_p - V_{sys} maps of the CO signal. The data quality is good enough to detect CO in individual transits, which is encouraging. Interestingly, each of the observations lead to a different peak offset in the K_p - V_{sys} map, with $\Delta K_p < 0$ km/s in transit 1, $\Delta K_p \approx 0$ km/s in transit 2, and $\Delta K_p > 0$ km/s in transit 3. Further data analysis will have to shed light on these differences.

H₂O signals

In the case of water, we also observe differences between the three transits. In transit 1, for example, we do not manage to detect water at all. In transit 2, the water signal is strongest around mid-transit (see Fig. A.2). In transit 3, the water signal is much stronger in the second half compared to the first half (see Fig. A.4). Again, further analysis should elucidate why the observations are discrepant, and to what extent the data-cleaning process affects the cross-correlation signal. Telluric lines are caused by water absorption in the Earth's atmosphere, so their removal through SVD could interfere with the planet signal.

Although we cannot detect water at $>5\sigma$ in the individual transits, the sum of the observations does lead to a significant detection. When combining all transits, we find a relatively strong (~ 20 km/s) positive offset in K_p , which is reminiscent of the peak offset found for water in WASP-76b by Sánchez-López et al. (2022). A positive peak offset could indicate that the Doppler shifts of the water lines are dominated by rotation, rather than atmospheric dynamics (e.g., Fig. 6.8).

OH signals

Based on three transits of WASP-121b, we do not find a significant detection of OH (see Fig. A.7).

Bibliography

- Parmentier V., et al., 2018, *A&A*, 617
 Sánchez-López A., Landman R., Mollière P., Casasayas-Barris N., Kesseli A. Y., Snellen I. A. G., 2022, *A&A*, 661, A78
 Sim C. K., et al., 2014, *Advances in Space Research*, 53, 1647

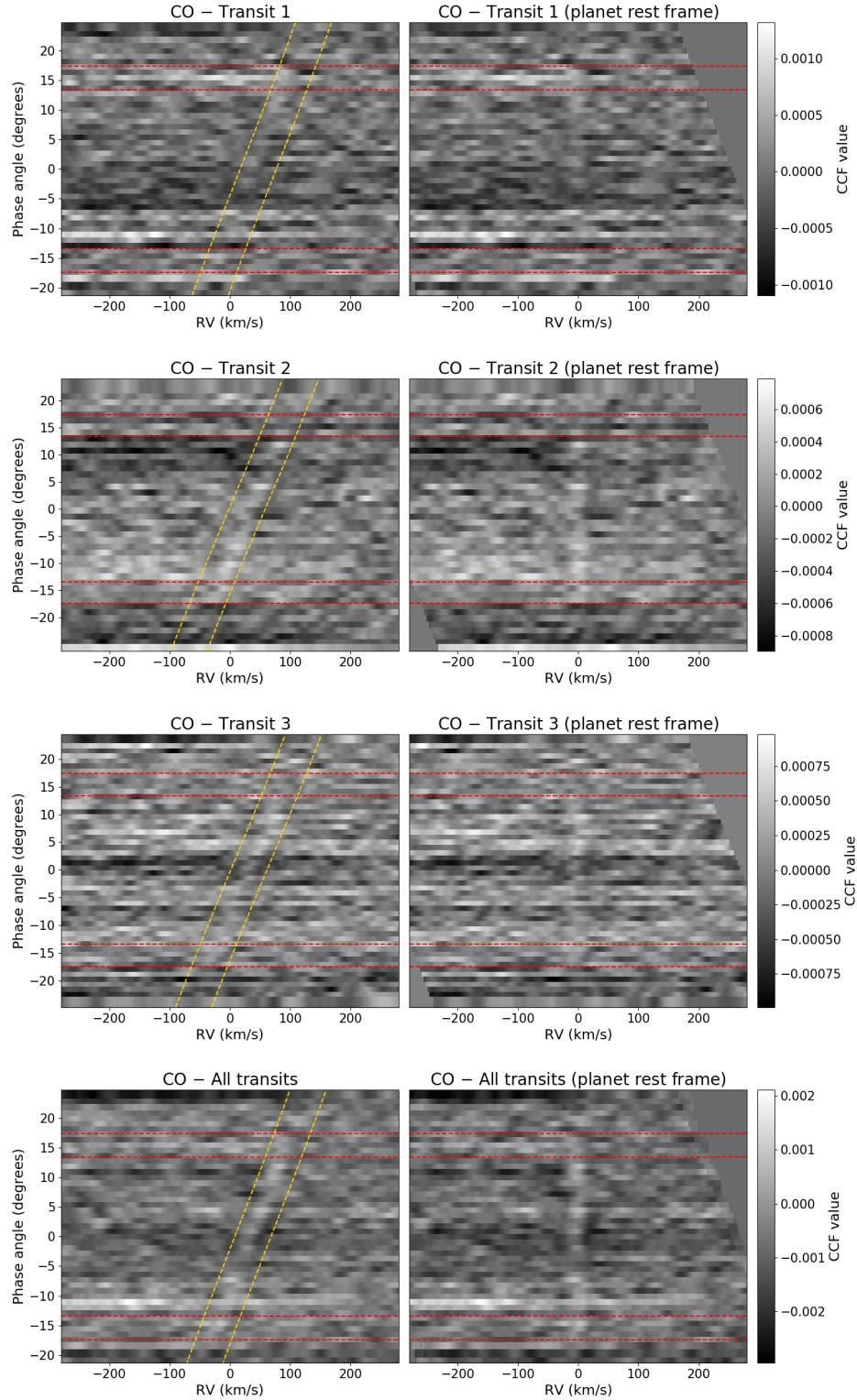


Figure A.1: CCF maps showing the CO absorption signal of WASP-121b. The top three rows depict the CCF maps for the individual transits, while the bottom row depicts the sum of the observations. In the left column, the observations are corrected for barycentric velocity, but not for the system velocity V_{sys} and the orbital motion K_p of the planet. This is why the planet signal manifests as a diagonal trail (between the yellow dashed lines) in the CCF map. In the right column, the data are transformed into the planetary rest frame, such that the planet signal appears as a vertical trail centered at zero. The red dashed lines mark the ingress (phase < 0) and egress phase (phase > 0) of the transit.

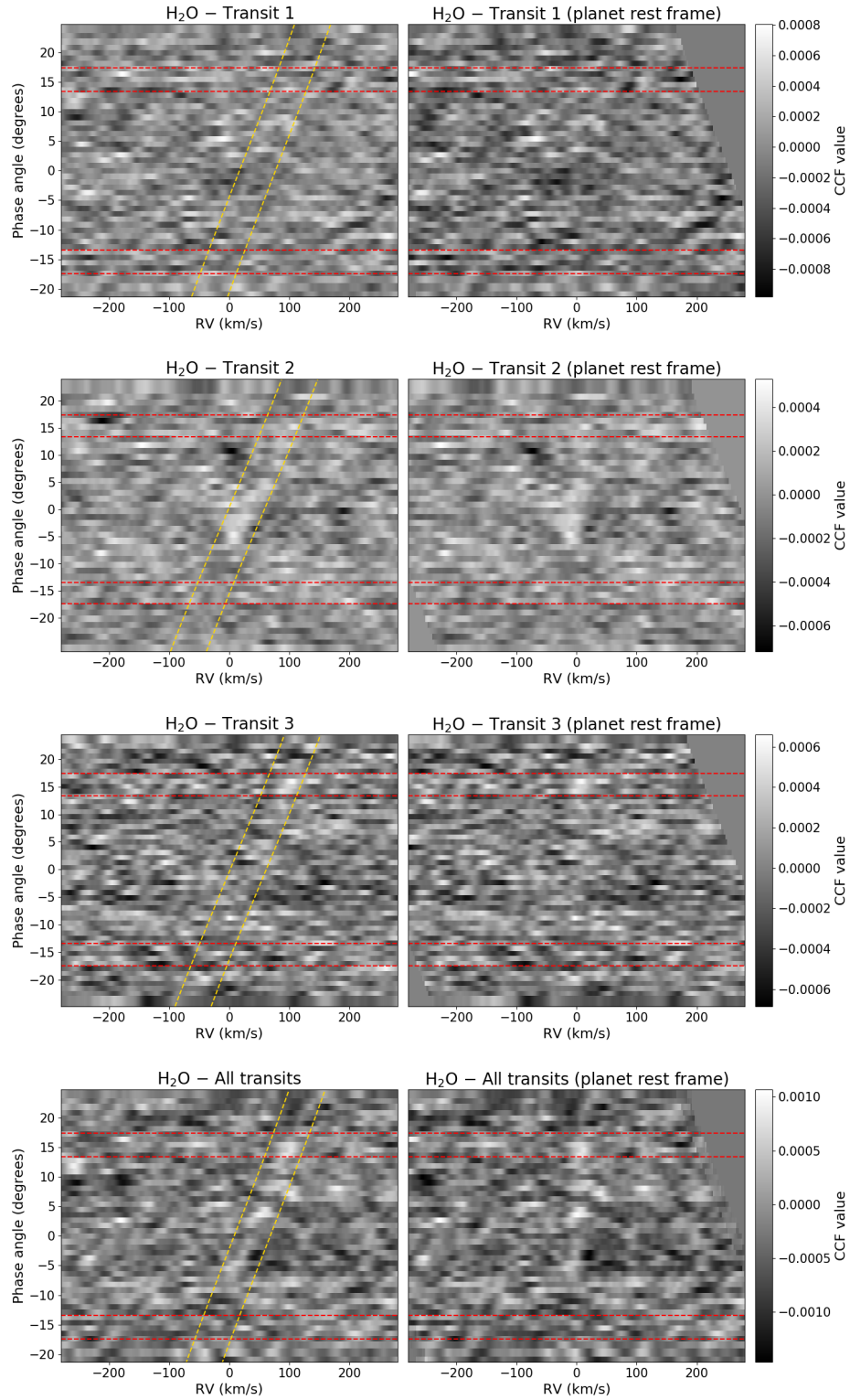


Figure A.2: Same as Fig. A.1, but for the water signal of WASP-121b.

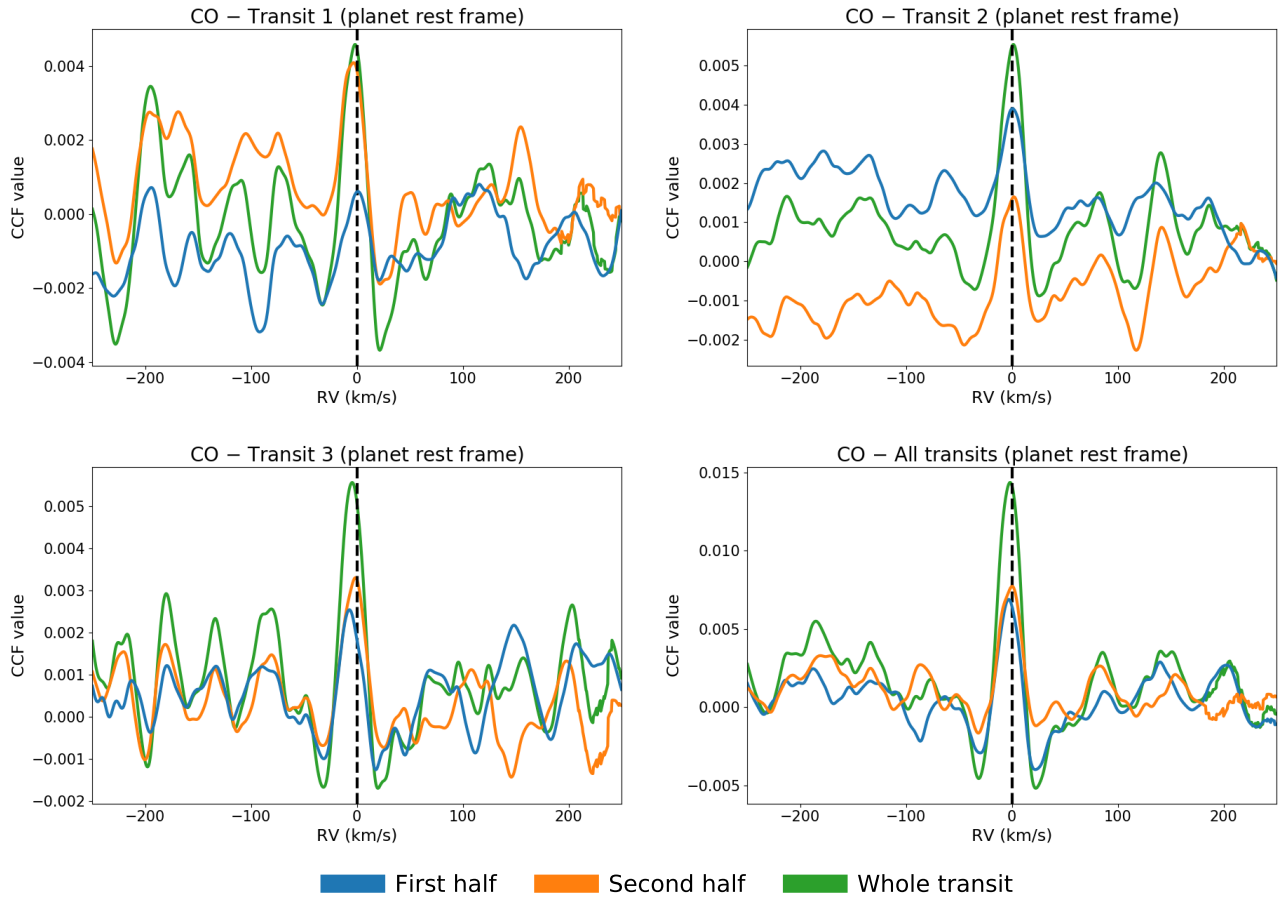


Figure A.3: CO absorption signals in the rest frame of WASP-121b. The 1D CCFs were obtained by summing the the 2D CCF maps (right column in Fig. A.1) along the phase axis. The panels in the top row and the bottom left depict 1D CCFs for the individual transits, while the bottom-right panel depicts the 1D CCFs for the sum of the observations. 1D CCFs were computed for the first half of the transit (blue), the second half of the transit (orange), and the whole transit (green).

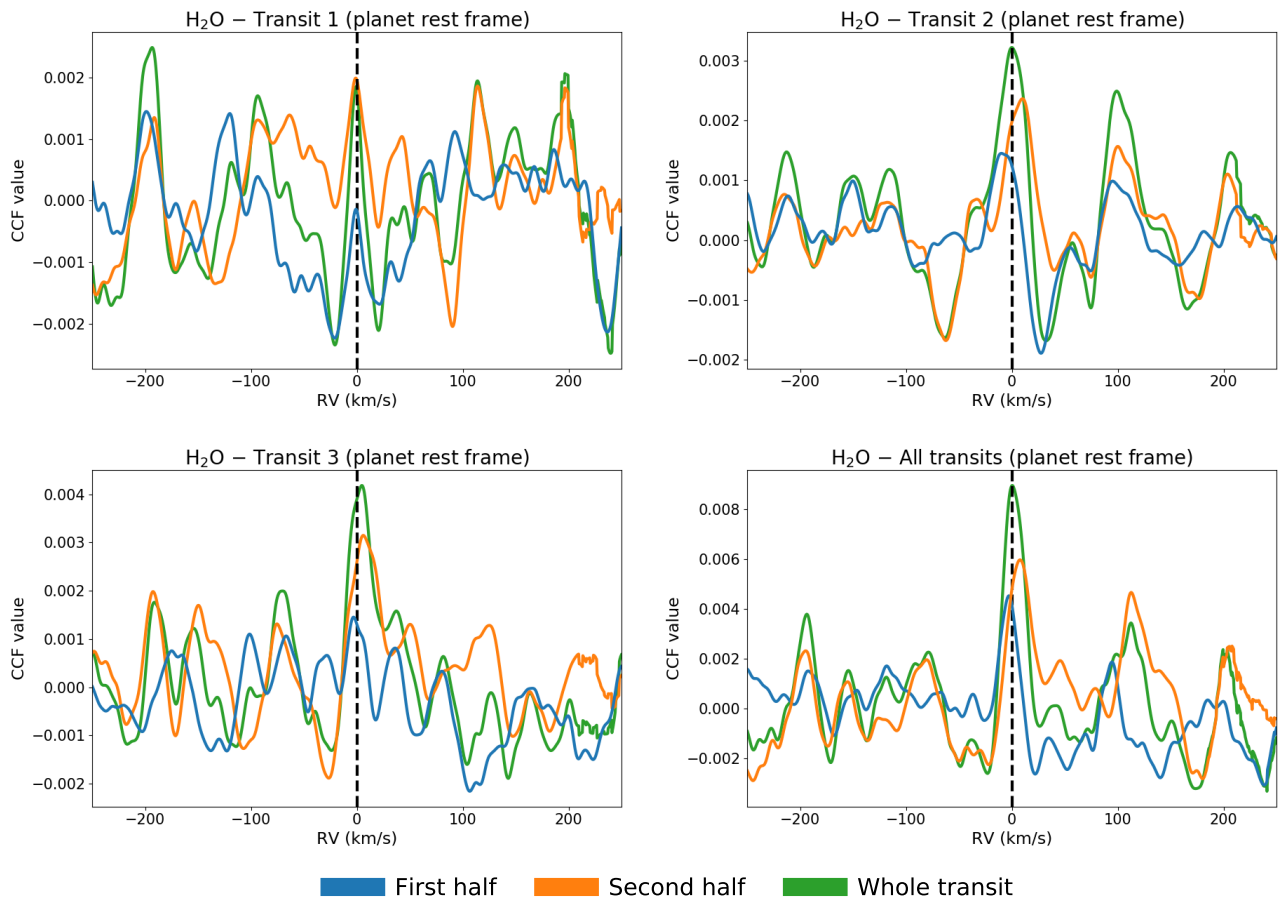


Figure A.4: Same as Fig. A.3, but now for the water signal of WASP-121b.

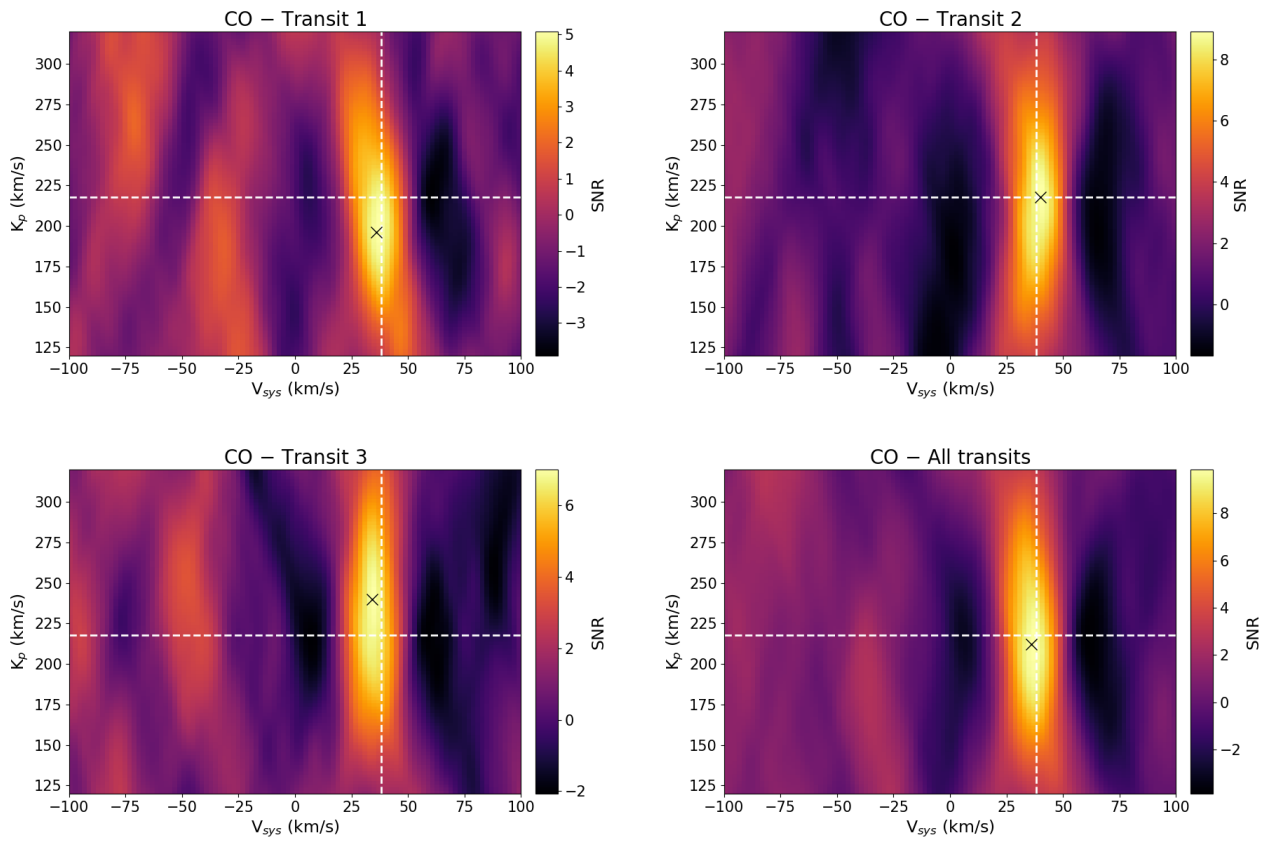


Figure A.5: K_p - V_{sys} maps showing the detection of CO in the atmosphere of WASP-121b. The panels in the top row and the bottom left depict K_p - V_{sys} maps for the individual transits, while the bottom-right panel depicts the K_p - V_{sys} map for the sum of the observations. When combining the three transits, we obtain a $>9\sigma$ detection for CO.

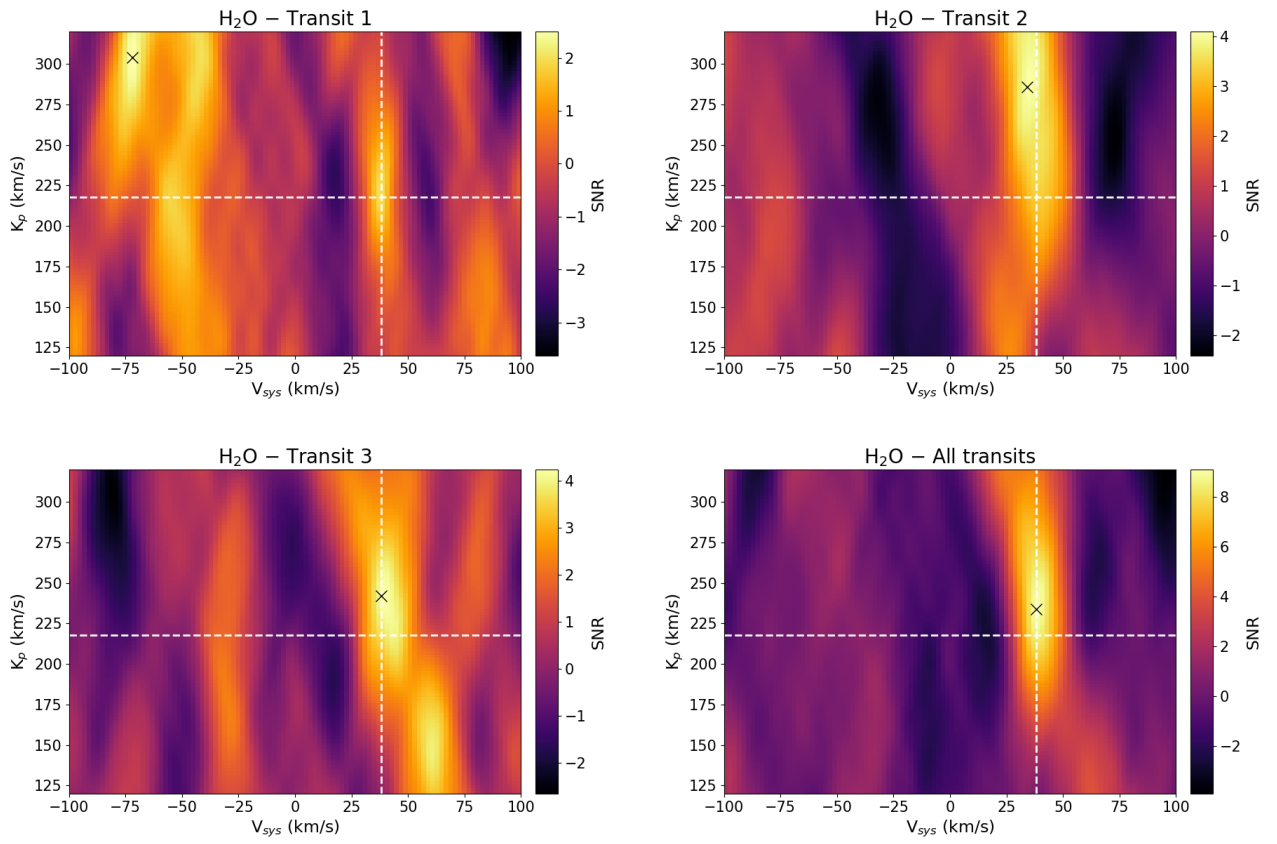


Figure A.6: Same as Fig. A.5, but now for water. When combining the three transits, we obtain a $>8\sigma$ detection for water.

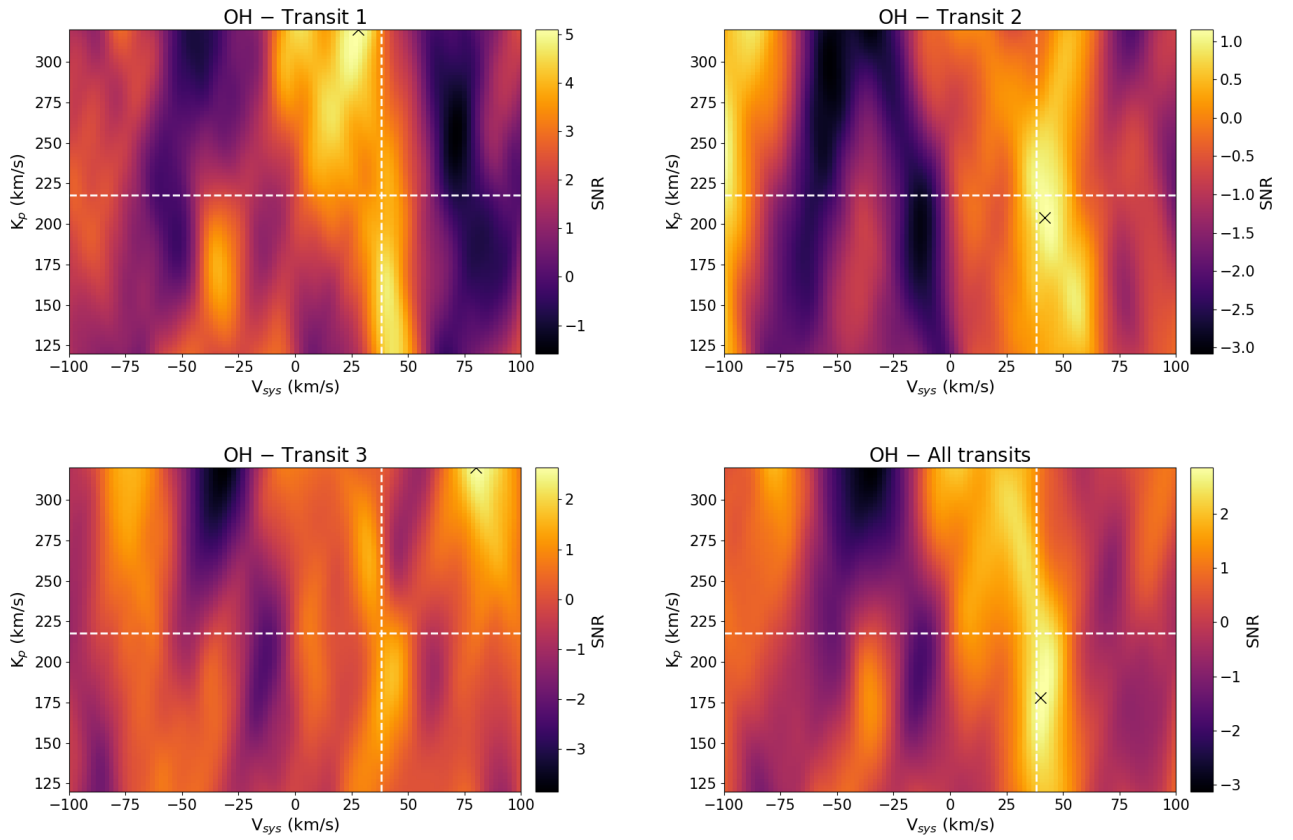


Figure A.7: Same as Figs. A.5 and A.6, but now for OH. We do not obtain a significant detection of OH when combining the three transits.

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Sekoah, I look back with pride on some of the dishes we cooked during lockdown, including pizza baguettes, pasta pesto with broccoli and pine nuts, and a five-story vegetarian lasagne. Defrosting the freezer was another highlight.

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