The Influence of H$_2$O Pressure Broadening in High-metallicity Exoplanet Atmospheres

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Abstract

Planet formation models suggest broad compositional diversity in the sub-Neptune/super-Earth regime, with a high likelihood for large atmospheric metal content ($\geq 100\times$ Solar). With this comes the prevalence of numerous plausible bulk atmospheric constituents including N$_2$, CO$_2$, H$_2$O, CO, and CH$_4$. Given this compositional diversity there is a critical need to investigate the influence of the background gas on the broadening of the molecular absorption cross sections and the subsequent influence on observed spectra. This broadening can become significant and the common H$_2$/He or “air” broadening assumptions are no longer appropriate. In this work, we investigate the role of water self-broadening on the emission and transmission spectra as well as on the vertical energy balance in representative sub-Neptune/super-Earth atmospheres. We find that the choice of the broadener species can result in a 10’s of parts-per-million difference in the observed transmission and emission spectra and can significantly alter the one-dimensional vertical temperature structure of the atmosphere. Choosing the correct background broadener is critical to the proper modeling and interpretation of transit spectra observations in high-metallicity regimes, especially in the era of higher-precision telescopes such as the James Webb Space Telescope.

Key words: molecular data – planets and satellites: atmospheres – planets and satellites: composition

1. Introduction

A primary goal of exoplanet science is the determination of basic planetary conditions. Transit spectrophotometry observations of planetary atmospheres offer a window into fundamental quantities such as climate and composition (e.g., Madhusudhan et al. 2016). Determining atmospheric composition is a necessary requirement for assessing the relative importance of various chemical processes (Moses 2014) and greatly assists in understanding planet formation by linking volatile inventory to protoplanetary disk processes (Pollack et al. 1996; Oberg et al. 2011; Madhusudhan et al. 2014; Cridland et al. 2016; Mordasini et al. 2016).

One of the key findings of the Kepler Mission (Borucki et al. 1997) is that a majority of exoplanets fall within this “warm sub-Neptune” regime ($\sim 2$–4 Earth radius, $T < 1000$ K; Fressin et al. 2013; Batalha 2014; Fulton et al. 2017). These planets have been an intense area of focus for transit spectra observations with the Hubble Space Telescope (HST; Fraine et al. 2014; Knutson et al. 2014; Kreidberg et al. 2014b). In addition, over the next decade they will serve as the link between Jovian worlds and terrestrial planets as well as being the most prolific population of planets to be found by the Transiting Exoplanet Explorer Satellite (Sullivan et al. 2015; Barclay et al. 2018; Kempton et al. 2018; Louie et al. 2018).

Planet formation, interior structure, and atmospheric chemistry modeling (Fortney et al. 2013; Moses et al. 2013; Lopez & Fortney 2014) suggest extreme compositional diversity within this subpopulation, with a high likelihood for large atmospheric metallicities ($\geq 100\times$ solar). Given this potential for compositional diversity, the assumption of “Jovian-like” H$_2$/He-dominated atmospheres may not always be appropriate. Instead, with currently measured atmospheric metallicities reaching as high as $\sim 300$–$1000\times$ solar (Fraine et al. 2014; Knutson et al. 2014; Kreidberg et al. 2014a; Line et al. 2014; Morley et al. 2017), molecules such as H$_2$O and CO$_2$ will become the dominant bulk constituents (Moses et al. 2013; Hu & Seager 2014).

Along with this diversity in composition comes numerous challenges in atmospheric modeling, from chemical modeling (Hu & Seager 2014) to cloud microphysics (Ohno & Okuzumi 2018) to 3D climate modeling (Kataria et al. 2014). Nearly all flavors of atmospheric modeling that aim to make observational predictions require radiative transfer computations. A key necessary ingredient in radiative transfer computations are the opacities, which for planets are dominated by the molecular absorption cross sections (hereafter ACS; Mihalas 1970). The ACS of a given molecule typically consist of billions of lines representing the ability of a molecule to absorb or emit photons. Each line has its own linewidth (or broadening) typically specified through the degree of thermal/Doppler and pressure broadening (Goody & Yung 1995). Pressure broadening is the net cumulative effect of interactions between the absorbing molecule in question (e.g., H$_2$O) and with its neighboring molecules (or bath gases, e.g., H$_2$, He) or by self-broadening (H$_2$O with itself). Much exoatmospheric relevant ACS focus, specifically broadening, has been Jovian-centric (e.g., H$_2$/He-dominated compositions and broadening; Freedman et al. 2008; Grimm & Heng 2015; Hedges & Madhusudhan 2016; Tennyson et al. 2016), which had been largely driven by the abundance of high-fidelity “hot-Jupiter” observations and carryover from brown dwarf modeling.

Exploration of pressure-broadening assumptions in exoatmospheres is not new (e.g., Grimm & Heng 2015; Hedges & Madhusudhan 2016). Hedges & Madhusudhan (2016) provide a comprehensive overview of the various pressure-broadening effects including resolution, line-wing cutoff, Doppler versus pressure, and more relevant to our investigation, an initial look at the impact of a broadener choice. They too explore the impact of H$_2$O versus H$_2$ broadening on the H$_2$O ACS, specifically over HST wavelengths, and found that the band-averaged ACS can change up to an order of magnitude. Our goal is to expand upon the work in Hedges & Madhusudhan (2016) to not only determine the influence of H$_2$O self-broadening on the H$_2$O ACS, but also as a function of water.
fraction, and more importantly, we quantitatively assess the integrated effect that the broadener choice has on the observable spectra as well as on the impact on the atmospheric vertical energy balance. This work is crucial to the proper interpretation of transit spectra observations in high-metallicity regimes expected of the sub-Neptune/Super-Earth population. In Section 2, we describe our data sources and how we compute the ACS and the transmission/emission spectrum and self-consistent modeling approach. In Section 3, we compare the impact of H$_2$O self-broadening with the standard H$_2$/He-broadening assumption. Finally, in Section 4, we discuss the implications and future prospects. We also make our newly computed water ACS grid for both broadeners publicly available.\textsuperscript{3}

2. Methods

In this initial investigation on the impact of non-H$_2$/He foreign broadening on transmission/emission spectra, we choose to focus on H$_2$O because: (1) H$_2$O is the most prominent absorber in exoplanet spectra due to its large abundance over a range of elemental compositions (Moses et al. 2013) and multiple strong absorption bands from the optical to far-infrared wavelengths and (2) it shows the largest sensitivity to choice of broadener when compared to other species (a factor of $\sim$7 increase in broadening when compared to H$_2$/He; Table 1).

The fundamental approach here is to compute the H$_2$O ACS being under different end-member scenarios, with the first the standard “Jovian-like” H$_2$/He broadening (H$_2$O@[H$_2$+He]) and the second, pure H$_2$O broadening (H$_2$O@[self]), which would be more appropriate for high-metallicity or all-steam atmospheres. We would then like to determine the spectral differences between H$_2$/He and self-broadening of H$_2$O in high-metallicity/all-steam atmospheres.

The computation of absorption cross sections relies upon the following input data: the rotation–vibration–electronic transitions, the molecular electronic energy states, and pressure-broadening coefficients (Barton et al. 2017). The aggregation of these data are often referred to as the “line list.”

2.1. Line Lists

The completeness and the accuracy of H$_2$O line list are essential, and they can be determined either through high-level quantum mechanics calculations or through spectroscopic laboratory measurements. The EXOMOL database contains the water BT2 line list (including transitions and electronic state data; Barber et al. 2006) for $T \lesssim 3000$ K, rotational quantum numbers (J) up to 50, and frequencies up to 30,000 cm$^{-1}$; a trimmed version of this line list is used in the HITEMP database (Rothman et al. 2010). The NASA Ames line list (Partridge & Schwenke 1997) is another ab initio source of water data that has more accurate line positions than BT2, but is less complete. Recently, there has been an attempt to improve the BT2 line list by refining the potential energy surfaces that resulted in raising J up to 72 and frequencies up to 40,000 cm$^{-1}$ (Polyansky et al. 2016). The pressure-broadening data provided by EXOMOL for H$_2$O are limited to H$_2$ and He. Complementary to ab initio studies, laboratory data integrated into the HITRAN database (Rothman et al. 1998) leverage high-resolution spectrometers to provide precision line positions and intensities. However, experimental HITRAN/HITEMP ACS data are mostly limited to the Earth-like environmental conditions (i.e., T < 350 K, P < 1 bar) with the dominant background broadener being “air” (N$_2$/O$_2$) and self-broadening (see Wilzewski et al. 2016 for recent improvements).

There is a clear gap in exoplanet relevant ACS, lying between the low-temperature air broadening provided by HITRAN (applicable to temperature terrestrial planetary atmospheres) and the high-temperature H$_2$/He broadening given by EXOMOL (applicable to H$_2$/He-dominated Jovian-like worlds). The high-metallicity, warm (sub-)Neptune/super-Earth subpopulation of exoplanets occupies a compositional regime between these two: neither pure H$_2$/He nor pure “air.” While the raw line data exist to compute these cross sections, this has yet to be done. For instance, EXOMOL has generated H$_2$O@[H$_2$+He] ACS using the BT2 line list for wavenumber ranges 100–30,000 cm$^{-1}$; however, their line-wing cut-off is not sufficiently large to accurately compute the ACS data in the spectral range of $\sim$100–1500 cm$^{-1}$ (6.7–100 $\mu$m; Barton et al. 2017). HITRAN/HITEMP do not provide the ACS of H$_2$O@[self]. Below, we describe how we compute our own ACS taking into account the composition-dependent broadening.

\begin{table}[h]
\centering
\begin{tabular}{|l|l|l|l|l|}
\hline
Absorber & Broadener & $\gamma_L$ [cm$^{-1}$/bar] & $\gamma_{L/He}$ & References \\
\hline
H$_2$O & Self\textsuperscript{a} & 0.3–0.54 & 7$x$ & 1, 2 \\
H$_2$/He\textsuperscript{b} & 0.05–0.08 & 1$x$ & 1 \\
CO$_2$ & air & 0.15–0.20 & 3$x$ & 1 \\
\hline
CH$_4$ & Self & 0.06–0.09 & 1.5$x$ & 3 \\
H$_2$/He & 0.05–0.08 & 1$x$ & 4 \\
H$_2$O & 0.06–0.09 & 1.5$x$ & 5 \\
CO$_2$ & 0.07–0.09 & 1.5$x$ & 6 \\
air & 0.02–0.07 & 1$x$ & 3 \\
\hline
CO$_2$ & Self & 0.08–0.12 & 1$x$ & 7 \\
H$_2$/He & 0.09–0.12 & 1$x$ & 8 \\
H$_2$O & 0.10–0.14 & 1.25$x$ & 9 \\
air & 0.05–0.08 & 0.5$x$ & 7 \\
\hline
CO & Self & 0.04–0.09 & 1$x$ & 10 \\
H$_2$/He & 0.04–0.08 & 1$x$ & 10 \\
H$_2$O & 0.07–0.1 & 1.5$x$ & 11 \\
CO$_2$ & 0.07–0.1 & 1.5$x$ & 11 \\
air & 0.05–0.07 & 1$x$ & 12 \\
\hline
\end{tabular}
\caption{Lorentzian Half-width coefficients $\gamma_L$ [cm$^{-1}$/bar] for Relevant Broadeners}
\end{table}

\textsuperscript{a} Relative to the average value of $\gamma_L$ of absorber @[H$_2$+He], e.g., H$_2$O@[H$_2$+He].

\textsuperscript{b} Denoted by H$_2$O@[self] in the text and figures.

\textsuperscript{c} Denoted by H$_2$O@[H$_2$+He] in the text and figures.

Notes. The focus of this work is on influence of H$_2$O self-broadening and H$_2$/He broadening on the H$_2$O absorption cross sections (in bold).

\textsuperscript{a} References.
(1) Brown et al. (2005), (2) Mashnik et al. (2016), (3) Smith et al. (2014), (4) Pine & Gabard (2003), (5) Delahaye et al. (2016b), (6) Lyulin et al. (2014), (7) Devi et al. (2016), (8) Padmanabhan et al. (2014), (9) Delahaye et al. (2016a), (10) Devi et al. (2002), (11) Hartmann et al. (1988), (12) Devi et al. (2012), and also data extracted from references in Table 3 of Hartmann et al. (2018) and from Gordon et al. (2017).

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Table 2

Grid and Computational Assumptions over which the H$_2^16$O Cross Sections Are Computed

| ACS   | Case 1: 85% H$_2$ 15% He | Case 2: 100% H$_2$ | H$_2$O | 100% H$_2$ | 10% H$_2$O | 30% H$_2$O | 100% H$_2$O |
|-------|---------------------------|---------------------|-------|--------|----------|----------|----------|
| $T$(K) |                           |                     |       |        |          |          |          |
| 400   |                           |                     |       |        |          |          |          |
| 900   |                           |                     |       |        |          |          |          |
| 1000  |                           |                     |       |        |          |          |          |
| 1100  |                           |                     |       |        |          |          |          |
| 1200  |                           |                     |       |        |          |          |          |
| 1300  |                           |                     |       |        |          |          |          |
| 1400  |                           |                     |       |        |          |          |          |
| 1500  |                           |                     |       |        |          |          |          |
| $P$(bar) |                             |                     |       |        |          |          |          |
| $10^{-6}$ |                         |                     |       |        |          |          |          |
| $3 \times 10^{-6}$ |                       |                     |       |        |          |          |          |
| $3 \times 10^{-5}$ |                       |                     |       |        |          |          |          |
| $3 \times 10^{-4}$ |                       |                     |       |        |          |          |          |
| $10^{-3}$ |                             |                     |       |        |          |          |          |
| $3 \times 10^{-3}$ |                       |                     |       |        |          |          |          |
| $10^{-2}$ |                             |                     |       |        |          |          |          |
| $3 \times 10^{-2}$ |                       |                     |       |        |          |          |          |
| $3 \times 10^{-1}$ |                       |                     |       |        |          |          |          |
| Resolution$^*$ |                             |                     |       |        |          |          |          |
| 100   |                           |                     |       |        |          |          |          |
| 1000  |                           |                     |       |        |          |          |          |
| Line-wing cutoff$^e$ |                             |                     |       |        |          |          |          |
| $P > 1$ |                           |                     |       |        |          |          |          |
| $P \leq 1$ |                           |                     |       |        |          |          |          |

Note. There are 270 $T$-$P$ combinations and two broadener choices (H$_2$+He versus H$_2$O). A variable wavenumber resolution is chosen to properly sample the Voigt widths at each given $T$-$P$ pair. Finer sampling result in negligible differences in the ACS.

$^e$ The Lorentz wing shape may not be appropriate out at such distances (Freedman et al. 2008).

2.2. Computation of Pressure-broadened H$_2^16$O Absorption Cross Sections

Molecules in the outermost layer of a given atmosphere (where $P < 10^{-6}$ bar) experience a negligible amount of interactions with their neighboring atoms or molecules due to the low collisional frequency and large collisional frequency (see the results section of Lyons et al. 2018). In this environment, Doppler broadening will be the dominant effect that forms the spectral line shape and will depend on the molecular mass, temperature, and spectral line position. Absorbing molecules start to collide and interact with background molecules more frequently as pressure increases in the lower layers in the atmosphere. These pressure-broadening interactions will increase as the pressure goes above $\sim 10^{-4}$ bar and will become the dominant broadening effect at $P > 10^{-1}$ bar. The pressure-broadening line profile can be represented effectively through Lorentzian line shape, and the associated Lorentzian linewidth $\Gamma_L$ will be calculated through Equation (1):

$$\Gamma_L = \sum_b (T/T_{ref})^{-n_F^b} \gamma_L^b P_b,$$

where $\Gamma_L^b$ is the Lorentzian coefficient, $P_b$ is the broadener’s partial pressure, $T_{ref}$ is the reference temperature (i.e., 296 K), $n_F^b$ is the temperature-dependence coefficient, and index $b$ represents the dependency of these parameters on the broadener (e.g., H$_2$, He, H$_2$; Hedges & Madhusudhan 2016). Kinetic theory predicts the $n_F^b = 0.5$. In typical broadened ACS spectra, both Doppler- and pressure-broadening line profiles convolve to generate a Voigt profile, and the Voigt linewidth $\Gamma_V$ (Olivero & Longbothum 1977) is represented by Equation (2):

$$\Gamma_V = 0.5346 \Gamma_L + \sqrt{0.2166 \Gamma_L^2 + \Gamma_G^2},$$

where $\Gamma_G$ is the Doppler linewidth. In this study, the pressure-broadened H$_2$O ACS data are computed for two set of broadeners: (1) 85% H$_2$ and 15% He using the J-dependent pressure coefficients provided the by EXOMOL group (Barton et al. 2017) and (2) 100% H$_2$O using the average value of available experimental self-broadening coefficients as J-independent data (Ptashnik et al. 2016). The water BT2 line list (Barber et al. 2006) is input into the EXOCROSS script$^4$ (Yurchenko et al. 2018) to model the full Voigt profile (Humlíček 1979) of every single line between 100 and 30,000 cm$^{-1}$ over a grid of applicable temperatures and pressures (Table 2). The spectral sampling resolution is optimized as a function of temperature, pressure, and pressure-broadening line profile.

Note. There are 270 $T$-$P$ combinations and two broadener choices (H$_2$+He versus H$_2$O). A variable wavenumber resolution is chosen to properly sample the Voigt widths at each given $T$-$P$ pair. Finer sampling result in negligible differences in the ACS.

$^e$ The Lorentz wing shape may not be appropriate out at such distances (Freedman et al. 2008).

$^4$ https://github.com/Trovemaster/exocross
Guillot 2010, Equations (24), (49)) and either 100% H₂O or 500× solar metallicity assuming thermochemical equilibrium molecular abundances. Second, we compute a self-consistent radiative–equilibrium atmosphere using the tools described in Arcangeli et al. (2018), Kreidberg et al. (2018), and Mansfield et al. (2018) to determine the impact of water broadening on the vertical energy balance and, in turn, on the observed spectra. We discuss our findings in the next section.

3. Results

3.1. Impact on Cross Sections

Figure 2 illustrates the effect of temperature, pressure, and water abundance on the difference between [self] and H₂O@H₂ broadening. The top panel shows the temperature effect at a fixed representative pressure of 1 mbar. At 1200 K (1 mbar) the lines are purely Doppler broadened resulting in little effect. The middle panel shows the influence of pressure at a fixed temperature. The Doppler cores are negligible by 1 bar. The bottom panel shows the impact of the relative weighting of self vs. H₂ broadening (e.g., composition dependence) at a fixed temperature and pressure. Absorption cross-section differences are largest in the pressure-broadened line wings, with pure [self] typically one order of magnitude larger. A factor of 5 in broadening difference occurs by the time the relative abundance of water reaches ∼30%. In general, [self] broadening becomes more important at higher pressures, cooler temperatures, and longer wavelengths due to the increased prominence of pressure broadening over Doppler broadening.

spectral subdivisions in such a way as to fully resolve the individual lines without undue computational burden (Table 2). Figure 1 illustrates the comparison between our adaptive resolution (see Table 2, i.e., 1 sampling point per half-width: 1/Γν or 2 sampling points per half-width: 2/Γν) with ultra-high sampling of 6 points per half-width (6/Γν) and with the EXOMOL computed ACS for H₂O@H₂ for P = 10⁻³ bar and T = 400 K.

2.3. Modeling the Impact on Transmission/Emission Spectra of Transiting Exoplanets

To assess the significance of the broadener assumption on exoplanet transmission/emission spectra, we use the CHIMERA code with our newly generated ACS (converted to 10 correlated-K coefficients; Amundsen et al. 2016) to model transit/eclipse spectra of a representative sub-Neptune-like planet (GJ1214b; Harpsøe et al. 2013; T_{eq} = 500–900 K). We first generate forward model spectra using both sets of ACS (H₂O@[self] and H₂O@H₂+He) given a fixed temperature-pressure profile (TP; http://exomol.com/data/data-types/xsec/H2O/1H2-16O/BT2/).
3.2. Direct Impact on Transmission/Emission Spectra

More practically, Figure 3 summarizes the key impact of \([\text{H}_2+\text{He}]\) versus \([\text{self}]\) broadening on the emission (top row) and transmission (bottom row) spectra of a typical sub-Neptune under the assumption of a pure-steam atmosphere (left column) and a 500× solar metallicity scenario (right column). Overall, we find that the relative differences (\(\Delta[\text{ppm}]\)) in the bottom panels in Figures 3(a), (b), (c), and (d) are quite large, 10 s to 100 s of ppm. These differences are well within the detectable range of both \(\text{HST}\) (Kreidberg et al. 2014b) and certainly the \(\text{James Webb Space Telescope (JWST)}\); e.g., Greene et al. 2016; Bean et al. 2018), especially for the anticipated windfall of such planets around bright stars (Sullivan et al. 2015).

In the all-steam atmospheres, emission differences (Figure 3(a)) are largest in the window regions (~4 μm, ~10 μm). The increased flux for the \([\text{H}_2+\text{He}]\)-broadened ACS is because of the lower opacity, permitting flux from deeper, hotter layers to emerge (for a fixed TP). The increased opacity due to the \([\text{self}]\) broadening obscures the deeper/hotter layers, resulting in lowered fluxes at those wavelengths. These differences are, of course, strongly dependent upon the

\([\text{H}_2+\text{He}]\)-broadened ACS near 6 μm. The top panel shows how broadening changes with temperature at a fixed pressure of 1 mbar. Differences are largest for cooler temperatures where pressure broadening becomes more important. The middle panel illustrates the impact of different pressures at a fixed temperature (725 K). Even at low pressures (1 μbar), pressure-broadening differences are still present in the line wings. The bottom panel shows the effect of varying water abundance on the combined \([\text{self}]+[\text{H}_2]\) broadening at a fixed temperature and pressure (725 K, 1 μbar). With pure self-broadening, differences in the line wings can approach an order of magnitude. For a ~30% mole fraction of water, the ACS is about 3–5× greater than pure hydrogen broadening. While not shown, these differences become larger at longer wavelengths and smaller at shorter wavelengths due to the relative importance of Doppler-to-pressure broadening.

\(\Delta[\text{ppm}]\) is a strong wavelength dependence.

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Figure 4. Comparison of the @self (blue) vs. @H2+He (red) broadening in self-consistent 1D thermochemical–radiative–equilibrium atmospheres for all-steam (left column: (a), (c), (e)) and 500× solar (right column: (b), (d), (f)) composition. The top row ((a), (b)) shows the derived radiative–equilibrium TP under each scenario. Thermal emission contribution functions averaged over representative bands (Cont. Func. 5–8, and 3.5–4.3 μm) for each broadening scenario are shown in panel (a). Panel (b) shows the thermochemical equilibrium mixing ratios along the @self TP for select species. Temperature differences can be up to 175 K (20%) in the pure-steam scenario and up to 70 K in the 500× solar scenario. The middle row ((c), (d)) shows the resultant secondary eclipse spectra and their differences below Δ. An additional emission spectrum (@H2+He, @self TP; green), is shown in panels (c) and (d) assuming the same TP as the @self scenario in order to decouple the effects of the radiatively adjusted TP from the broadening differences. The bottom row ((e), (f)) shows the resulting cloud free transmission spectra and relative differences. An additional transmission spectrum (@H2+He, @self TP; green), is shown in panels (e) and (f) assuming the same TP as the @self scenario in order to decouple the effects of the broadening and scale height change due to TP variation. Spectral differences are on the order of 30–40 ppm in transmission but are much less in emission (~60 ppm) when compared to Figures 3(a), (b) due to the radiative adjustment of the TP.
temperature structure within the atmosphere. As these spectra assume a fixed TP there is a difference in net radiated flux, which will most certainly have an influence on the radiative balance and thermal structure in the atmosphere, as discussed in Section 3.3.

Transmission spectra tell a similar, albeit less dramatic, story with relative differences of $\sim 60$ ppm across the shown wavelength range. The “linear-like” slope in the differences with wavelength is due to the frequency dependence of Doppler-to-pressure broadening.

The effects at high metallicity (500× solar; Figure 3, right column) are less extreme (tens of ppm) due to the reduced abundance of H$_2$O (10%–20%) and the significant abundances of additional opacity sources (mainly CO$_2$, CO, CH$_4$, and H$_2$/He). Furthermore, due to the reduced impact of H$_2$O@[self] broadening (Figure 2), we expect an approximate (comparing 1 mbar line wings) reduction of 3–5× to $\sim 10$ ppm in the transmission spectra.

3.3. Impact on Self-consistent 1D Atmosphere

Figure 4 shows the impact of self-broadening on the 1D radiative balance (and subsequent observational effects) of a $\sim 550$ K planet under the all-steam and 500× solar scenarios. The @[self] broadening results in $\sim 100$–180 K hotter temperatures below the $\sim 1$ mbar level and $\sim 60$ K cooler above for the all-steam scenario (Figure 4(a)). More intuitively, the increased @ [self] mean opacity “shifts” the averaged thermal “$T = 1$” level to a $\sim 3\times$ lower pressure in the all-steam scenario. This shift is readily seen in the band-averaged contribution functions (Figure 4(a)). A similar, but lesser, effect is seen in the 500× solar metallicity scenario (up to $\sim 70$ K) because the water abundance is lower by a factor of $\sim 5$ (Figure 4(b)). The radiative response of the TP to the integrated flux differences (up to 40% for steam and 10% for 500× solar; green versus red curves in Figures 4(c), (d)) between the @[self] versus @[H$_2$/He] acts to reduce the emission spectrum differences, however, to a still detectable tens of ppm (Figures 4(c), (d)).

The transmission spectra (Figures 4(e), (f)) show comparable differences (30–40 ppm) to the 500 K scenario from Figures 3(c), (d). However, there are now two effects taking place that create the transmission differences. The first is the scale height effect due to the differences in the TP (@[H$_2$/He]@[self], H$_2$O TP), and the second, as before, is the broadening difference. Both effects contribute equally to the overall differences in the transmission spectra. Despite the self-consistent adjustment of the TP, differences in both emission and transmission are still above detectable levels (tens of ppm).

4. Conclusions

The determination of unbiased exoplanet atmosphere properties (e.g., temperatures and abundances) from their spectra necessarily requires a full accounting of potential model inadequacies. The aim of this work was to assess the role of the background gas broadener under plausible bulk super-Earth/(sub-)Neptune atmospheric compositions. Specifically, we focused on the differences between the typically assumed H$_2$/He broadening and water self-broadening on the water vapor absorption cross sections.

From our analysis we arrive at the following key points:

1. Absorption cross-section differences between water self-broadening and the standard assumed H$_2$/He broadening are up to an order of magnitude in the pressure-broadened line wings (similar to Hedges & Madhusudhan 2016) and are noticeable over a range of applicable temperatures and pressures.
2. The influence of self-broadening is composition dependent and nonlinear, with $\sim$half of the difference achieved by water mole fractions of $\sim$30% for a representative temperature and pressure.
3. Transmission and emission spectra differences for representative sub-Neptune atmospheres range between a few tens of ppm up to hundreds of ppm, depending upon wavelength, temperature, and water abundance. These differences are not negligible considering currently achieved HST precisions of $\sim$15 ppm and possible precisions as low as a few ppm for JWST. Differences will vary depending upon additional parameters like temperature gradient (for emission), planet-to-star radius ratio, and scale height. The wavelength dependence of these differences are unlikely to be mimicked by other atmospheric processes.
4. The assumption of water self-broadening (or lack thereof) can have a significant impact on the 1D vertical energy balance, with temperature differences of up to 180 K in pure-steam atmospheres (or a half-a-decade lower pressure shift in the emission levels) and tens of K in high-metallicity atmospheres.

This work is certainly not an exhaustive exploration of all possible broadening (Table 1) or planetary atmosphere conditions. However, it serves to illustrate that the broadener composition can have a nonnegligible impact on the observables and continues to illustrate the importance and key role of laboratory data on planetary atmosphere modeling (Fortney et al. 2016).

5. Supplementary Data

The computed pressure-broadened H$_2$O absorption cross-section (ACS) data for both self-broadening (or H$_2$O@[self]) and H$_2$/He (or H$_2$O@[85%H$_2$ + 15%He]) are publicly available at [doi:10.5281/zenodo.2459971] (see Table 2 for more details).

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References

Amundsen, D. S., Mayne, N. J., Baraffe, I., et al. 2016, A&A, 595, A36
Arcangeli, J., Désert, J.-M., Line, M. R., et al. 2018, ApJL, 855, L30
Barber, N. R., Tennyson, J., Harris, G. J., & Tolchenov, R. N. 2006, MNras, 368, 1087
Barclay, T., Pepper, J., & Quintana, E. V. 2018, ApJS, 239, 2
Barton, E. J., Hill, C., Yurchenko, S. N., et al. 2017, JQSRT, 187, 453
Batalha, N. M. 2014, PNAS, 111, 12647
Bean, J. L., Stevenson, K. B., Batalha, N. M., et al. 2018, PASP, 130, 114402
Borucki, W. J., Koch, D. G., Dunham, E. W., & Jenkins, J. M. 1997, in ASP Conf. Ser. 119, Planets Beyond the Solar System and the Next Generation of Space Missions, ed. D. Soderblom (San Francisco, CA: ASP), 153
Brown, L. R., Chris Benner, D., Malathy Devi, V., Smith, M. A., & Toth, R. A. 2005, JMoSt, 742, 111
Cridland, A. J., Pudritz, R. E., & Alessi, M. 2016, MNras, 461, 3274
Delahaye, T., Landsheere, X., Pangu, E., et al. 2016a, JMS, 326, 17
Delahaye, T., Landsheere, X., Pangu, E., et al. 2016b, JQSRT, 173, 40
Devi, M. V., Benner, C. D., Smith, M., et al. 2012, JQSRT, 113, 1013
Devi, V. M., Benner, D. C., Smith, M. A., Rinsland, C. P., & Mantz, A. W. 2002, JQSRT, 75, 455
Devi, V. M., Benner, D. C., Sung, K., et al. 2016, JQSRT, 177, 152
Fortney, J. J., Robinson, T. D., Domagal-Goldman, S., et al. 2016, arXiv:1602.06305
Fraine, J., Deming, D., Benneke, B., et al. 2014, Natur, 513, 526
Freedman, R. S., Lustig-Yaeger, J., Fortney, J. J., & Frey, J. D. 2014, ApJS, 214, 25
Freedman, R. S., Marley, M. S., & Lodders, K. 2008, ApJS, 174, 504
Fressin, F., Torres, G., Charbonneau, D., et al. 2013, ApJ, 766, 81
Fulton, B. J., Petigura, E. A., Howard, A. W., et al. 2017, AJ, 154, 109
Goody, R. M., & Yung, Y. L. 1995, Atmospheric Radiation : Theoretical Basis (2nd ed.; Oxford: Oxford Univ. Press)
Gordon, I., Rothman, L., Hill, C., et al. 2017, JQSRT, 203, 3
Gordon, S., & Mcbride, B. J. 1994, NASA RP-1311, https://www.grc.nasa.gov/WWW/CEAWeb/RP-1311.htm
Greene, T. P., Line, M. R., Montero, C., et al. 2016, ApJ, 817, 17
Grimm, S. L., & Heng, K. 2015, ApJ, 808, 182
Guillot, T. 2010, A&A, 520, A27
Hartmann, J. M., Hansen, S. M., & Innis, T. C. 2013, A&A, 549, A10
Hartmann, J. M., Rosenmann, L., Perrin, M. Y., & Taine, J. 1988, ApOpt, 27, 3063
Hartmann, J.-M., Tran, H., Armante, R., et al. 2018, JQSRT, 213, 178
Hedges, C., & Madhusudhan, N. 2016, MNras, 458, 1427
Hu, R., & Seager, S. 2014, ApJ, 784, 63
Humlíček, J. 1979, JQSRT, 21, 309
Katari, T., Showman, A. P., Fortney, J. J., Marley, M. S., & Freedman, R. S. 2014, ApJ, 785, 92
Kempton, E. M.-R., Bean, J. L., Louie, D. R., et al. 2018, PASP, 130, 114401
Knutson, H. A., Benneke, B., Deming, D., & Homeier, D. 2014, Natur, 505, 66
Kreidberg, L., Bean, J. L., Desert, J. M., et al. 2014a, ApJL, 793, 2
Kreidberg, L., Bean, J. L., Desert, J.-M., et al. 2014b, Natur, 505, 69
Kreidberg, L., Line, M. R., Bean, J. L., et al. 2015, ApJ, 814, 66
Lopez, E. D., & Fortney, J. J. 2014, ApJ, 792, 1
Louie, D. R., Deming, D., Albert, L., et al. 2018, PASP, 130, 044401
Lyons, J., Herde, H., Stark, G., et al. 2018, JQSRT, 210, 156
Lyulin, O. M., Petrova, T. M., Solodov, A. M., Solodov, A. A., & Perevalov, V. I. 2014, JQSRT, 147, 164
Madhusudhan, N., Agúndez, M., Moses, J. I., & Hu, Y. 2016, SSRv, 205, 285
Madhusudhan, N., Amin, M. A., & Kennedy, G. M. 2014, ApJL, 794, L12
Mansfield, M., Bean, J. L., Line, M. R., et al. 2018, AJ, 156, 10
Mihalas, D. 1970, Series of Books in Astronomy and Astrophysics (San Francisco: Freeman, c1970)
Mordasini, C., van Boekel, R., Mollière, P., Henning, T., & Benneke, B. 2016, ApJ, 832, 41
Morley, C. V., Knutson, H., Line, M., et al. 2017, AJ, 153, 86
Moses, J. I. 2014, RSPTA, 372, 20130073
Moses, J. I., Line, M. R., Visscher, C., et al. 2013, ApJ, 777, 34
Öberg, K. I., Murray-Clay, R., & Bergin, E. A. 2011, ApJL, 743, L16
Ohno, K., & Okuzumi, S. 2018, ApJ, 859, 34
Olivo, J., & Longbothum, R. 1977, JQSRT, 17, 233
Padmanabhan, A., Tzanetakis, T., Chanda, A., & Thomson, M. 2014, JQSRT, 133, 81
Partridge, H., & Schwenke, D. W. 1997, IChPh, 106, 4618
Pine, A. S., & Garbuz, V. 2016, JQSRT, 177, 92
Pollack, J. B., Hubickyj, O., Bodenheimer, P., et al. 1996, Icar, 124, 62
Polansky, O. L., Ovsyannikov, R. I., Kyuberis, A. A., et al. 2016, JMS, 327, 21
Ptashnik, I. V., McPheat, R., Polansky, O. L., Shine, K. P., & Smith, K. M. 2016, JQSRT, 177, 92
Rothman, L., Gordon, I., Barber, R., et al. 2010, JQSRT, 111, 2139
Rothman, L., Rinsland, C., Goldman, A., et al. 1998, JQSRT, 60, 665
Smith, M. A., Benner, D. C., Predoi-Cross, A., & Malathy Devi, V. 2014, JQSRT, 133, 217
Stevenson, K. B., Bean, J. L., Seifahrt, A., et al. 2014, AJ, 147, 161
Sullivan, P. W., Winn, J. N., Berta-Thompson, Z. K., et al. 2015, ApJ, 809, 77
Tennyson, J., Yurchenko, S. N., Al-Refaie, A. F., et al. 2016, JMS, 327, 73
WitzeWSKI, J. S., Gordon, I., E., Kochanovad, R. V., Christian, H., & Laurence, S. R. 2016, JQSRT, 168, 193
Yurchenko, S. N., Al-Refaie, A. F., & Tennyson, J. 2018, A&A, 614, A131