

Generating and Characterizing Terrestrial Exoplanet Atmospheres through Computational Modeling and Observations

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Dissertation Abstract

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The field of exoplanetary science and astrobiology entered a golden era when the first exoplanet around a Sun-like star, 51 Pegasi-b, was discovered in 1995. In the last 30 years alone, the number of confirmed exoplanets has grown from 1, to nearly 6000. With the recent launch of JWST, the community is once again on the precipice of rapid growth and discovery. For the first time, JWST has enabled the potential observation of high mean molecular weight atmospheres on terrestrial exoplanets, enabling the foremost searches for atmospheric biosignatures and habitability indicators on Earth-sized exoplanets. However, given technological limitations, these surveys are constrained to terrestrials with M dwarf hosts, in what has become colloquially known as "The M-dwarf Opportunity". While these planets may be Earth-sized, they exist in radically different stellar and system environments than our home planet. The extreme stellar activity, extended pre-main sequence phase, and close proximity of the habitable zone to M dwarf hosts leads to radiative challenges for planetary companions. Moreover, the long lifetimes and strong gravitational interactions in M dwarf systems suggest many of these planets are tidally locked, potentially leading to steep temperature gradients across the surface, powerful winds, and in extreme cases, atmospheric collapse. Given the vast range of evolutionary pathways possible for terrestrial planets in these systems, robust evolutionary modeling is becoming increasingly vital to interpreting JWST observations, predicting observational discriminants, identifying likely false positive biosignatures, and connecting the extant atmospheres discovered to likely evolutionary his-

tories.

The body of research described in this dissertation is intended to prepare the scientific community to analyze data, select subsequent observations, and connect observational results to likely evolutionary histories of terrestrial exoplanets. Furthermore, we demonstrate that tenuous (~ 0.1 bar) atmospheres are possible and may be likely for irradiated M dwarf planets, sustained by constant geochemical outgassing against extreme expected stellar-driven escape. In this work, we focus on the high priority TRAPPIST-1 system of seven Earth-sized planets, which has been the target of early and ongoing JWST campaigns. Through this work, we provide comprehensive analyses of past and present atmospheric evolution on the TRAPPIST-1 planets, along with suggestions for future observations. However, while we apply our methods to TRAPPIST-1, the tools, data pipelines, and experimental methodology we develop are broadly applicable to general terrestrial exoplanet characterization, which has been identified as a NASA priority research area through their selection of JWST DDT time and the conception of the Habitable Worlds Observatory. To predict and constrain the generation and evolution of secondary atmospheres in this work, we employ computational models for hydrodynamic thermal atmospheric escape, atmospheric photochemistry, planetary climate, JWST noise modeling, JWST observation planning, and line-by-line radiative transfer. Additionally, we develop and test several approaches to modeling pipelines to achieve varying balances of computational efficiency, simulation detail, and statistical rigor. Through our extensive use of computational modeling, we characterize the past and present atmospheric evolution of the TRAPPIST-1 planets, and provide a real world example of how to conduct terrestrial exoplanet characterization with JWST.

We begin by considering the early evolution of the TRAPPIST-1 system as a whole, driven by the extreme radiation from the host star's pre-main sequence phase. During this time, we find that all 7 planets undergo periods of hydrodynamic thermal atmospheric escape which typically lead to desiccation on the interior planets and water loss of up to nearly 10 Earth oceans on planets in the habitable zone. Furthermore, by connecting this work with the

pioneering JWST observations of TRAPPIST-1b and c, we show that atmospheric oxygen on the interior planets could provide an upper limit on the initial water content for all planets in the system of approximately 8 Earth oceans, suggesting the outer planets may have retained surface water when entering the habitable zone. With this important historical context of water loss, we find that oxygenated atmospheres are theoretically justifiable TRAPPIST-1 system.

With the likely history of volatiles on these planets informed by the first project in this work, we then look to current observing efforts to constrain the plausible extant atmospheres on the TRAPPIST-1 planets. As JWST observations continued, it became clear that thin oxygen-dominated atmospheres are among the only atmospheric scenarios still consistent to $<1\sigma$ for TRAPPIST-1b, c, and d observations. Moreover, significant upcoming observation time allocated to TRAPPIST-1e motivates the need to understand potential atmospheric compositions on the habitable zone planets that could be uncovered by future data.

Guided by the currently available and future observations, we also conduct comprehensive parameter sweeps of realistic outgassing, surface deposition, and top-of-atmosphere escape rates to identify self-consistent atmospheres for all 7 planets. For TRAPPIST-1b, c, d, and e, we identify several atmospheric compositions and climate profiles that are still consistent with current data. For the outer planets of the system, we provide the community with atmospheric spectra that represent a range of environmental archetypes that may be useful in planning and justifying upcoming observing campaigns. Finally, we apply advanced Bayesian nested sampling algorithms with a photochemical model to select realistic boundary conditions for TRAPPIST-1c and fit for the source and sink rates that best match current JWST thermal emission observations with quantified statistical uncertainty. Overall, we support the conclusion that thin (~ 1 mbar – 0.5 bar) O_2 -dominated atmospheres provide the best fitting atmospheric solution for the emission data of TRAPPIST-1c.

This body of work is one of the first ever examples of how to combine observations, atmospheric models, and statistical methods to discern constraints on planetary source and sink

fluxes for terrestrial exoplanets. It pioneers methodology for how to best fit self-consistent atmospheric profiles to data, which has broad implications for atmospheric retrieval in the future. For the first time, we show that tenuous atmospheres can be generated and maintained by geochemical outgassing on the irradiated M dwarf planets of the TRAPPIST-1 system, despite the expected high atmospheric escape rates.

DEDICATION

To my parents, Christina and Anthony Gialluca.

I began my journey in astronomy at 16 years old. From the moment I looked through my first telescope, to the moment I published my first research paper, you were there. You have always supported me in everything I've done in life, and there has never been a moment where I wondered if you were proud of me.

You've supported me emotionally, loudly, and financially, and there has never been a moment where I thought I would have to face the challenges in my life alone if I needed you. You gave me the space and freedom to make my own mistakes and find my own path, but the love and support to know I wouldn't have to do it alone.

This achievement belongs as much to you as it does to me, because without you I would not be the woman I am today, and I certainly would not have had the privilege or resources to seek a doctorate.

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CHAPTER 1

INTRODUCTION

The Earth is a small stage in a vast cosmic arena.

– Carl Sagan, 1994

With the discovery of over 6000 exoplanets in the last 30 years, the increasing number of possible alien worlds has invigorated the search for life in the universe and instilled widespread interest in exoplanet atmosphere and environment characterization. This interest is especially reflected by the most recent NASA Astrophysics Decadal Survey ([National Academies of Sciences, Engineering, and Medicine et al., 2021](#)), which placed a specific focus on the discovery and spectroscopic characterization of at least 25 habitable zone Earth-like exoplanets orbiting Sun-like stars through the conception, development, and launch of a future flagship mission: the Habitable Worlds Observatory (HWO). In the near-term, the flagship JWST space telescope, launched in 2021, has provided the community with the first opportunity to conduct spectral analysis and atmospheric characterization of Earth-sized rocky exoplanets; however, due to observing considerations and technological limitations, these observations are limited to Earth-sized planets with M dwarf host stars, which has become colloquially known as ‘The M dwarf Opportunity’. The environments of M dwarf planetary companions, particularly those in the habitable zone, may vary significantly from what we see in the Solar System, but nevertheless, they offer us the first opportunity to test our models and understanding of terrestrial exoplanet evolution on real data. As it is currently unknown if M dwarf systems can support life, this is also the first time we are able to test our concepts of planetary habitability and the ‘cosmic shoreline’, which is that combination of stellar and planetary characteristics and distance from the star that allows a planet to retain an atmosphere ([Zahnle & Catling, 2017](#)). With JWST, the community finally has an opportunity to explore best practices and workflows for interpreting observations to understand the nature of a terrestrial exoplanets. This critical time in our field will provide experience, tools, and know-how for upcoming missions dedicated specifically to the search for life on exoplanets, such as HWO.

To interpret new data on terrestrial exoplanets, we will need theoretical models that predict environmental properties and the impact of key processes on observable characteristics.

Given the complex geophysical, photochemical, climate, and star-planet interactions that take part in shaping a terrestrial planet’s environment, designing computational models to match observational data is inherently challenging. These models must capture all of the necessary physical processes and their interplay, while being careful to avoid overfitting in areas of evolution that are unknown.

Furthermore, while we can quantify the fit of a given atmospheric model to the available observations, the ability to inter-compare model runs with different planetary characteristics, and say which compositions are overall more likely than others, requires a statistical sample of models. Generating a large enough modeling suite to yield a statistically significant result often requires extensive computation time, and may be immediately unfeasible if a single run of a particular model is very time-consuming. This constrained computation time may also restrict the physical complexity of available models to interpret observations. As we move into a new era of exoplanetary observation and discovery, we must address these modeling challenges, refine our data analysis techniques, and use a variety of tools to maximize the information return of limited datasets.

Here I explore different applications and coupling of time-evolution, photochemical-climate, geochemical, aeronomy, and radiative transfer models in conjunction with the evolving landscape of available observations for a primary M dwarf system of interest: the 7-planet TRAPPIST-1 system. We first consider how the likely early evolution of the system as a whole will shape the probable mantle and atmospheric compositions of the planets at present-day; this knowledge of past evolution can help identify the best observations to target for characterization, and illuminate processes that can lead to oxygen-rich atmospheres without the presence of life.

To address and overcome the considerable computational challenges facing terrestrial exoplanet characterization, we then use a high performance computing (HPC) approach to generate models of the TRAPPIST-1 planetary atmospheres, and identify a suite of atmospheric cases consistent with JWST data from multiple observing campaigns. This work builds on an existing photochemical-climate model to provide the first terrestrial exoplanet code that can self-consistently calculate atmospheric composition and pressure, and also take into account the balance of outgassing and escape rates. The idea of self-consistency is a primary theme of this work, it is when a model allows the composition and physical state of an atmosphere to be driven by the incident spectrum of the host star, accounting for all of the known laws of physics and chemistry as well as the interactions between them; when an atmospheric model is ‘self-consistent’ it is approaching our best approximation of what a real atmosphere could be. Using our novel code, we show how these environmental modeling pipelines can not only be self-consistent in photochemical-climate space, but also in outgassing-escape space. Allowing the surface pressure to vary further allows us to provide the first theoretical study demonstrating the feasibility of M dwarf terrestrials to generate and sustain tenuous (<1 bar) secondary atmospheres at present day, and to potentially support habitable environments.

Finally, we combine techniques from all previous work into a Bayesian nested sampling algorithm which takes a statistical approach to matching models of a grid of atmospheric states to available observations. Similarly to a retrieval, this approach quantifies statistical confidence in simulated environments and spectra by matching observations to atmospheric compositions but, unlike a retrieval, this approach also considers the chemical and physi-

cal plausibility of the environment being modeled. This modeling approach considers full photochemical-climate calculations that are consistent with the spectrum of the host star, allowing it to target constraints on the origin and loss processes (sources and sinks) of atmospheric constituents and the overall surface pressure of an atmosphere. By combining statistical modeling techniques and physically realistic planetary models, we are able to fit self-consistent spectra to observations and infer photochemical profiles, and even interior properties, with quantified uncertainty.

The tools, techniques, and results used to study and explore the nature of the TRAPPIST-1 planets in this dissertation not only further our understanding of a terrestrial exoplanet system of great community interest, they also pioneer a practical example of how to characterize the environments of Earth-sized planets in alien star systems. The following subsections of this introduction provide the background on the transmission and emission spectroscopy used to gather the data we make comparisons to, JWST observational strategy, the exciting TRAPPIST-1 system under study, and challenges to terrestrial planet characterization in the era of observation, that provide context and are needed to understand the impact and significance of the research results presented in this dissertation. The structure of this dissertation is further outlined in §5.

1 JWST & Observational Techniques for Probing Terrestrial Exoplanet Atmospheres

In 1995, two major events occurred in the astronomy community: the first exoplanet orbiting a main sequence star was discovered (Mayor & Queloz, 1995), and a mission concept known as the Next Generation Space Telescope (NGST) was recommended by the “AURA HST and Beyond” committee (Dressler et al., 1996). At that time, NGST was the result of nearly a decade of prior work from many professionals (Illingworth, 2016), and by the end of 2002, NGST would go by a new name: JWST. Although JWST was initially conceived to unveil the nature of the earliest universe, as the field of exoplanet science grew in parallel with the mission’s development, a new use case and design driver for JWST quickly emerged: it would become an engine for exoplanet characterization, and the first mission capable of observing the atmospheres of Earth-sized exoplanets (Gialluca et al., 2021; Lustig-Yaeger et al., 2019a; Meadows et al., 2023; Wunderlich et al., 2019).

Given the vast distances separating us from our stellar neighbors, exoplanet characterization relies on remote sensing techniques, such as photometry and spectroscopy. JWST predominantly uses the techniques of transmission and emission spectroscopy and photometry at near- and mid-infrared wavelengths to study exoplanets (e.g., Pontoppidan et al., 2022; Sabelhaus & Decker, 2004), although it can also use coronagraphy to block out a star’s radiation and directly image young, large planets that are distant from their stars (e.g., Boccaletti et al., 2022; Girard et al., 2022). Enabled by technology demonstrations with the Nancy Grace Roman Space Telescope (Bailey et al., 2023), the future HWO will use even more sensitive coronagraphy to directly image Earth-like planets around nearby Sun-like stars, and measure their reflected light spectra (e.g., Feinberg et al., 2026; McElwain et al., 2025). Here we provide an overview of the physics behind transmission and emission

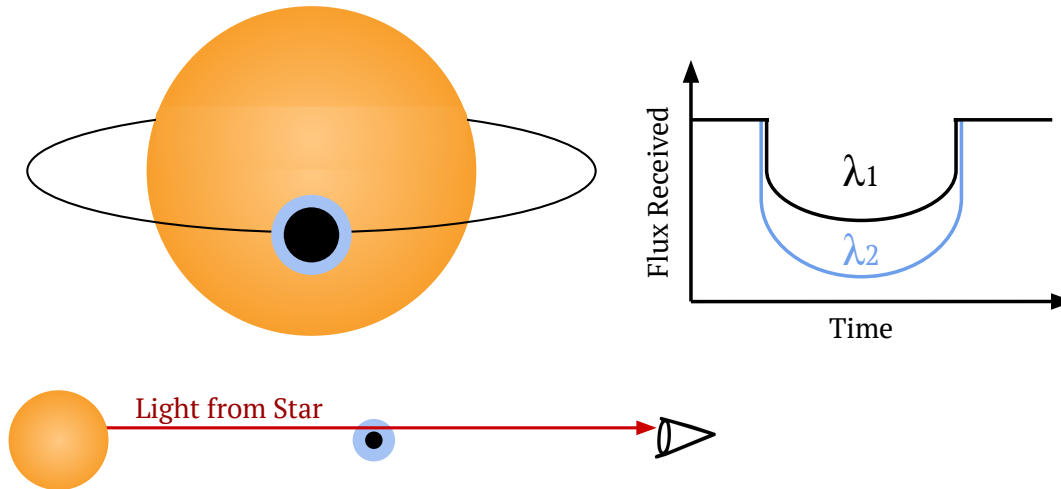


Figure 1.1: A diagram showing the transit of a planet across its host when transmission spectroscopy may be conducted. The top left image shows the system from the observers point of view, and the bottom illustration shows a side view of how the light from the host passes through the planetary atmosphere and arrives at the observer. The top right plot illustrates how the flux received by the observer will be lower when observing a wavelength (λ_2) in which the atmosphere is opaque, versus a wavelength (λ_1) in which the atmosphere is transparent.

spectroscopic observations of planetary atmospheres, which will comprise the observational datasets used throughout this dissertation.

Transmission spectroscopy of terrestrial exoplanets may be conducted when the planet transits in front of its host star (Brown, 2001; Charbonneau et al., 2002; Seager & Sasselov, 2000). This scenario is illustrated by Figure 1.1, when the planet is between its host and the observer, light passing through the planetary atmosphere can be recorded and studied. At this time, the reduction in brightness seen (compared to the star alone) will be proportional to the radius of the planet divided by that of the star squared. This reduction in brightness is referred to as the ‘transit depth’. However, when the companion possesses an atmosphere, the atmospheric constituents will cause the opacity to vary as a function of wavelength (Seager & Sasselov, 2000). This means that the planet will appear ‘larger’ at wavelengths where significant absorption occurs. The top right plot of Figure 1.1 illustrates this process, at wavelength λ_1 the atmosphere is transparent and the transit depth is shallow, from only the solid body of the planet (shown in black); however, at wavelength λ_2 , the atmosphere (shown in light blue) is opaque, and the transit depth is deeper indicating atmospheric absorption. Observing the light passing through the planetary atmosphere thus allows the identification of absorption features, and subsequently their attribution to molecules of interest via a retrieval framework (e.g., Lustig-Yaeger et al., 2023a). A retrieval framework typically employs a radiative transfer routine as its forward model to constrain the abundance of gases that will

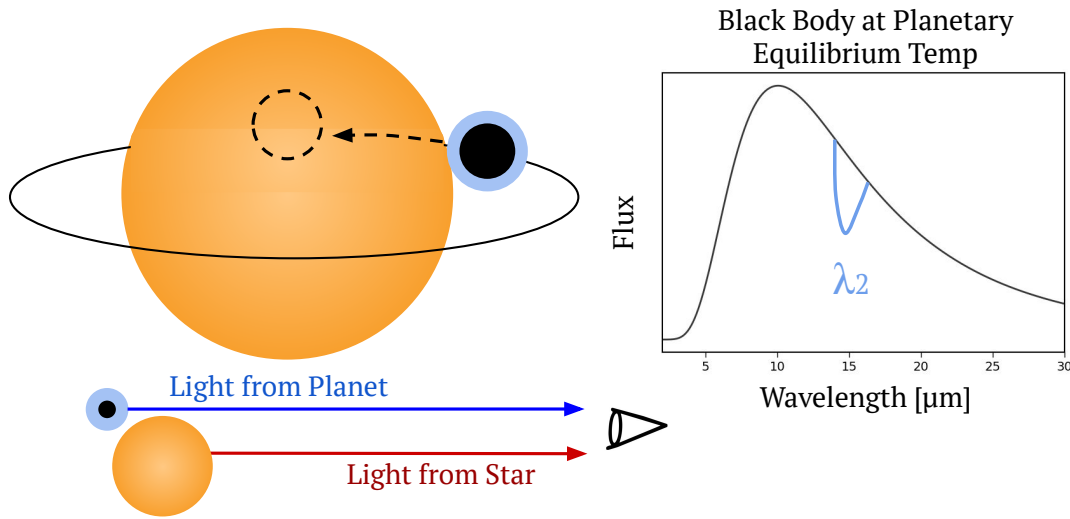


Figure 1.2: A diagram showing the secondary eclipse, when a planet transitions behind its host star, during which time emission spectroscopy can be conducted. The top left image shows this transition from the point of view of the observer, and the bottom illustration shows a side on view where the observer can record the combined light from the star plus the planet before the planet disappears behind its host. Once the planet disappears, the light solely emitted from the star can be recorded and subtracted from the combined profile to yield just the light from the planet itself. The top right plot shows an example of an emission absorption feature: when an atmosphere is present that is opaque at a specific wavelength (λ_2), the emission or flux observed is lower than the expected equilibrium temperature black body curve.

best lead to absorption or emission features seen across an observed spectrum; in this way, retrievals constrain which species may be present in an atmosphere based on the absorption observed as a function of wavelength.

Emission spectroscopy may be conducted when the planet is about to pass behind its host star, and the light emitted solely by the host star when the planet disappears may be subtracted from the combined star-planet light, yielding just the contribution of planetary emission (plus light reflected off the atmosphere) (Charbonneau et al., 2005; Deming et al., 2005). This scenario is illustrated by Figure 1.2, in which the combined star-planet light is observed just prior to the planet passing out of sight behind its host. If the planet was airless, a near ideal black body spectrum may be observed in emission, which is set by the temperature of the surface. However, when an atmosphere is present, the emitted flux observed may deviate from the expected blackbody for an airless planet for two different reasons. The first reason is atmospheric absorption, in which constituents may attenuate or block emission from the surface; at these optically thick wavelengths, the emission seen in observation will come from a layer of the atmosphere at greater altitude where radiation has an unobstructed path to escape. This emitting layer in the atmosphere may be hotter or colder

than the surface, leading to measured emission that deviates from an airless body’s expected black body spectrum. Similarly to transmission, these absorption or emission features in the emission spectrum correspond to specific gases and may allow atmospheric composition to be inferred. An absorption feature in a planetary emission spectrum is illustrated by the top right plot of Figure 1.2, in which the wavelength where the atmosphere is opaque (λ_2) produces an observed flux much lower than the planetary equilibrium temperature black body curve (shown in black).

The second pathway in which observed emission may be lower than expected for an airless body when an atmosphere is present is because atmospheres redistribute heat around the planet. This second possibility is particularly important for tidally locked planets, such as the majority of those with M dwarf hosts. When a planet is airless and tidally locked, the dayside is constantly being heated. However, if an atmosphere is present, heat generated on the dayside can be redistributed to the nightside of the planet, effectively lowering the temperature of the dayside surface which is the target of emission observations.

Because of the temperature dependence of emission spectroscopy, this technique provides information on the temperature at the surface and/or at various altitudes in the atmosphere. Planetary thermal emission can be observed in a variety of approaches including photometry, spectroscopy, and phase curves. Photometry and spectroscopy are very similar, just differing in that photometry considers a single bandpass while spectroscopy observes the emission across a range of wavelengths. In other words, observing thermal emission in a single photometric band will yield one data point at a wavelength of interest, or one can observe emission across a broad wavelength range (i.e., spectroscopy). Thermal phase curves are similar to photometry, except the idea is to observe the planetary emission in a wavelength of interest at every point in the planet’s orbit. For a tidally locked planet, this allows one to discern how the emission in a given bandpass (as a proxy for temperature) varies from the day to nightside of the body. This can directly probe the degree to which heat is being redistributed from the dayside through atmospheric motion.

Transmission and emission spectroscopy of Earth-sized planetary atmospheres is exceptionally challenging due to the extreme size and temperature contrast of a terrestrial planet to its host star; thus, JWST is limited to M dwarf systems, the smallest and coldest of all main sequence stars (e.g., [Gialluca et al., 2021](#); [Lustig-Yaeger et al., 2019a](#); [Wunderlich et al., 2019](#)), which provide the largest spectroscopic signals (e.g., [Brown, 2001](#); [Deming et al., 2005](#); [Tarter et al., 2007](#)). The signal size of both transmission and emission features scales inversely with the square of the host star radius (e.g., [Brown, 2001](#); [Deming et al., 2005](#)); while there is also a dependence on the planetary radius (squared in the case of emission), Earth-size planets definitionally remain the same size regardless of their hosts, thus smaller host stars lead to maximized signal. Furthermore, emission observations also scale with the ratio of the planetary to stellar blackbody function; again, if one is searching for an exoEarth with a temperate climate and a surface temperature near ~ 280 K, reducing the stellar temperature serves to maximize this temperature scale law. For example, the radius ratio squared of the Earth-Sun is $\sim 8 \times 10^{-5}$, and if we replace the Sun with the well-known M dwarf star TRAPPIST-1 ($R_* \sim 0.12 R_\odot$, $T_* \sim 2566$ K, [Agol et al., 2021](#)), this square radius ratio becomes $\sim 6 \times 10^{-3}$, implying a signal increase of $\sim 75\times$ in transmission for the Earth around TRAPPIST-1 versus the Sun. Outside of the tails of the stellar blackbody functions, the additional signal from the temperature dependence leads to a total signal increase of

$\gtrsim 160\times$ when observing an Earth around TRAPPIST-1 versus the Sun.

2 M dwarf Systems & Their Planetary Evolution

While true Earth-Sun twins are not accessible for characterization with JWST, Earth-sized terrestrial planets in M dwarf systems are. However, due to the challenging radiative environment of M dwarfs, it is still unknown if these stars may harbor habitable environments on their planetary companions. Because of the low stellar luminosity, the habitable zone of an M dwarf is located much closer to the star than for any other type of main sequence star. This close proximity leads to both gravitational challenges such as likely tidal locking, which can lead to synchronous rotation and extreme temperature gradients (Barnes, 2017; Lobo et al., 2023; Yang et al., 2014), and radiative challenges such as heightened XUV radiation (e.g., Lamers & Levesque, 2017) and increased planetary cross-section to prevalent flaring and proton events (e.g., Hawley et al., 2014; Howard et al., 2023; Segura et al., 2010).

In addition to these present-day hazards, there are also evolutionary challenges, as M dwarfs experience an extended pre-main sequence (PMS) phase, during which time the star is at its brightest as it contracts to its main sequence size (Baraffe et al., 2015). For all stars, the high energy XUV evolution is tied to the bolometric luminosity. When a star enters the PMS phase, it begins as XUV saturated, during which time they are emitting their maximum XUV energy which is set as a fraction of the bolometric luminosity (Lamers & Levesque, 2017). The duration over which a star remains XUV saturated depends on its rotation and spin down rate (Johnstone et al., 2021). The saturation threshold is inversely related to the convective turnover rate, which is decreasing over time, causing the rotation required to maintain saturation to increase (Johnstone et al., 2021). Simultaneously, the star is spinning down, and eventually the saturation threshold becomes higher than the rotation, leading to the star's exit from the XUV saturation phase, and an overall drop in the XUV energy produced (Johnstone et al., 2021). For a Sun-like star, both the PMS and XUV saturation phase are on the order of tens of millions of years (Baraffe et al., 2015), but as a star gets smaller, these evolutionary phases take longer. For a small star like an M dwarf, the saturation threshold is much lower, and they also spin down much slower, meaning the M dwarf's XUV saturation phase lasts much longer than larger stars (Johnstone et al., 2021). Additionally, a star's bolometric luminosity (tied ultimately to the net XUV produced) is decreasing as a star contracts to the main sequence; since an M dwarf is the least massive main sequence star, it has the slowest contraction and thus the slowest rate of change for bolometric luminosity. Overall, M dwarf stars provide XUV output that may be orders of magnitude brighter than on the main sequence, and this XUV saturation can last a billion years or more (e.g., Baraffe et al., 1998; Baraffe et al., 2015; Dotter et al., 2008; Lamers & Levesque, 2017; Reid & Hawley, 2013). This means that M dwarf planetary companions often have completed their formation processes long before the end of the PMS phase, and are thus subjected to extreme XUV radiation in excess of the runaway greenhouse limit – even for planets that will evolve into the main sequence star's habitable zone (HZ) (Luger & Barnes, 2015).

Despite these harsh stellar conditions, M dwarf planets may be able to generate and sustain secondary atmospheres, if they have a reliable source of outgassed material. Past work has

demonstrated that outgassing may provide sufficient material to replenish an atmosphere (Thomas et al., 2025), allowing it to build up against high expected escape rates ($\sim 10^{26} - 10^{30} \text{ s}^{-1}$; Brain & Hinton, *private comm.*, Dong et al., 2018) driven by radiation from the parent M dwarf. Furthermore, the bulk composition of outgassed material (H_2O , CO_2 , SO_2) may be a function of the planetary surface pressure (Gaillard et al., 2021), further indicating that atmospheres and geochemical processes are intimately tied and should be considered as a whole system when assessing the likelihood of and nature of planetary atmospheres.

Although we have an opportunity with JWST to observe terrestrial planets with M dwarf hosts, these atmospheres and environments may be significantly different than our solar system terrestrials. In addition to single target JWST General Observer (GO) campaigns (e.g., Greene et al., 2023; Lim et al., 2023), the community has also composed a more extensive concerted effort to explore M dwarf terrestrials through JWST Director Discretionary Time (DDT). The Rocky Worlds JWST DDT program is now investing 500 hours of observation time to surveying Earth-like planets on the inner edge of their host star’s habitable zones (Redfield et al., 2024). This program is meant to constrain the existence of an M dwarf ‘cosmic shoreline’, a relationship between planetary escape velocity and instellation that defines the possibility of atmospheric retention (Zahnle & Catling, 2017). While these observations provide a vital window into the nature of these terrestrials, observations must be interpreted to uncover that nature, which requires well-vetted physical models. Extensive and diverse computational modeling is needed in tandem with observations to identify plausible atmospheric compositions and properties, and likely evolutionary histories. Moreover, these JWST observations now offer the first chance to test our theories of habitability and water retention in one of the harshest stellar environments.

3 The TRAPPIST-1 Planets

By the end of 2017, a bountiful seven planets were known to orbit an extremely small ($\sim 0.12 R_\odot$), nearby (~ 12 parsecs) M8V dwarf, TRAPPIST-1 (Gillon et al., 2016, 2017; Luger et al., 2017), which is an excellent target for terrestrial exoplanet characterization. The TRAPPIST-1 planets are all very close to their star and have short orbital periods (1.5 – 18 days; Agol et al., 2021) allowing the rapid observation of numerous transits and secondary eclipse events. Not only is the size, luminosity, and proximity of TRAPPIST-1 ideal for planetary spectroscopy, but also the delicate resonance structure and planet-planet interactions of the system are highly conducive to transit timing variation (TTV) analysis. TTV observations measure the inconsistencies in intervals between transits, that are produced by gravitational interactions between the planets in the system (Agol & Fabrycky, 2018). TTV analysis provides refined timing (e.g., transit time, orbital period) and planetary masses, which, when combined with sizes from transit, allow planetary density constraints that inform internal composition and structure (Agol et al., 2021; Grimm et al., 2018). These observed parameters provide inputs for theoretical models and can enable precise predictions of transits and secondary eclipses for observing campaigns (Agol et al., 2021).

The abundance of Earth-sized planets distributed both interior to, within, and exterior to the TRAPPIST-1 habitable zone also provides an excellent opportunity to study stellar-driven atmospheric evolution as a function of distance. As a late-type M dwarf star,

TRAPPIST-1 is expected to have undergone an extended PMS phase (Baraffe et al., 1998; Birky et al., 2021), providing heightened XUV to its planetary companions and potentially driving extreme thermal atmospheric escape in the system’s early history (Gialluca et al., 2024; Luger & Barnes, 2015). In this body of work, we demonstrate how this hydrodynamic thermal escape period may desiccate planetary companions and abiotically produce significant and detectable O_2 —providing context for the past atmospheric evolution of the system as a foundation for interpreting observations of the planets in the era of JWST.

Driven by the observational accessibility of the system, the existence of 3 – 4 habitable zone planets, and the mystery of planetary evolution driven by such an alien environment, community interest in observing the TRAPPIST-1 system has flourished. Prior to JWST, observing campaigns have been executed by the Hubble Space Telescope, Spitzer, K2, and several ground-based facilities (Bourrier et al., 2017a; Burdanov et al., 2019; de Wit et al., 2016; De Wit et al., 2018; Delrez et al., 2018; Ducrot et al., 2018, 2020; Gillon et al., 2016, 2017; Luger et al., 2017); a useful review of these pre-JWST observations is covered in Turbet et al. (2020a). Unfortunately, given the significant challenges to observing the atmospheres of Earth-sized exoplanets, observations prior to JWST were primarily only able to rule out cloud-free hydrogen-dominated atmospheres (e.g., De Wit et al., 2018; Wakeford et al., 2019), and constraints on high mean molecular weight atmospheres, as well as the presence of aerosols, remained elusive.

The first JWST observations of the TRAPPIST-1 system were emission observations of the two hottest, innermost planets, that ruled out denser atmospheres but allowed for the possibility of a thin atmosphere, or no atmosphere at all. The first $15\mu\text{m}$ MIRI imaging observations of the inner-most planet, TRAPPIST-1b (Greene et al., 2023), revealed a sweltering surface ($T_B = 503 \pm 27$ K) consistent with the planet’s expected equilibrium dayside temperature ($T_{eq,day} = 508$ K). The direct interpretation of this measurement is that there is no absorption in TRAPPIST-1b’s $15\mu\text{m}$ band, and seemingly no evidence for heat redistribution. This led many to conclude that the innermost planet in the system likely did not possess an atmosphere (Greene et al., 2023; Ih et al., 2023). In emission, this $15\mu\text{m}$ measurement was soon followed up with a $12.8\mu\text{m}$ observation which threw the airless interpretation into question, as the measured brightness temperature was considerably lower than the expected equilibrium dayside temperature (Ducrot et al., 2025). While some explanations have been offered for the low $12.8\mu\text{m}$ emission on TRAPPIST-1b (including surface compositions or haze layers) (Ducrot et al., 2025), no robust self-consistent study has explained this measurement at present. Additionally, $15\mu\text{m}$ phase curve measurements have been taken for TRAPPIST-1b (Gillon et al., 2026), but these observations, showing large day to night temperature gradients indicative of thin or no atmosphere, have not significantly changed our understanding of the nature of TRAPPIST-1b at this time.

Similarly to TRAPPIST-1b, the first observation of the second planet in the system, TRAPPIST-1c, was a $15\mu\text{m}$ MIRI photometric measurement, which showed a brightness temperature of 380 ± 31 K, 1.7σ below the expected equilibrium dayside blackbody at $T_{eq,day} = 430$ K (Zieba et al., 2023). This difference conclusively ruled out a thick, CO_2 -rich atmosphere for TRAPPIST-1c, as may have been expected for a Venus analog, but still allowed the planet to have a thin atmosphere, or one lacking in significant greenhouse gases like CO_2 (Lincowski et al., 2023; Zieba et al., 2023). While $12.8\mu\text{m}$ observations of TRAPPIST-1c are not yet public, $15\mu\text{m}$ phase curve observations of the planet have helped to disfavor higher

pressure (>1 bar) steam atmospheres (Gillon et al., 2026).

While emission observations are only possible for the hottest, closer-in planets, transmission observations are possible for cooler planets also, and have been conducted and published for TRAPPIST-1b, c, d, and e (Allen et al., 2025; Espinoza et al., 2025; Glidden et al., 2025; Lim et al., 2023; Piaulet-Ghorayeb et al., 2025; Radica et al., 2025). Although transmission observations for the outermost planets have also been taken, they have not been made public at the time of this dissertation. Unfortunately for the community, all transmission observations of TRAPPIST-1 to date have displayed extreme stellar contamination, including flares, star spots, and faculae due to both activity during transit observations, as well as stellar inhomogeneities along the path of the transit (Howard et al., 2023; Lim et al., 2023; Rackham et al., 2018). This has made observational errors typically several factors larger than most molecular spectral features (Lim et al., 2023; Radica et al., 2025), making interpretation extremely difficult, and while some thick atmospheres with significant absorbers (e.g., clear-sky Venus analogs) have generally been ruled out, this current lack of precision means that many atmospheric cases remain possible in the context of transmission data.

4 Challenges to Terrestrial Planet Characterization

As JWST has provided the first opportunity to observe terrestrial exoplanet atmospheres, the community is now uncovering unresolved challenges that impede our ability to definitively characterize these planetary environments. These challenges include observational issues, such as stellar contamination (e.g., Lim et al., 2023; Rathcke et al., 2025) and data reduction (e.g., Gillon et al., 2026; Wakeford et al., 2019), as well as modeling issues, such as the lack of self-consistent photochemistry and climate calculations in simulated data and retrieval frameworks (e.g., Barstow & Heng, 2020; Tremblay et al., 2020). The work in this dissertation focuses primarily on the modeling challenges to terrestrial exoplanet characterization, but we also provide a summary of observational challenges for the reader’s edification.

Prior to JWST, the transit light source effect was already identified as a potential challenge to observation, particularly for M dwarfs like TRAPPIST-1 (Rackham et al., 2018). This contamination occurs because the disk of the star is not spatially resolvable in observation, so stellar inhomogeneities cannot be mapped across the surface. When a planet then transits its host star, it is unknown if the planet is passing in front of star spots and/or faculae, or if they remain unocculted. Thus, the planet may block more of the overall stellar flux than expected, affecting the inferred size of transmission features attributed to the planetary atmosphere.

Both the transit light source effect and the impact of stellar flares are now known to be present in transmission observations of the TRAPPIST-1 planets, producing large errorbars in the data (Allen et al., 2025; Espinoza et al., 2025; Glidden et al., 2025; Lim et al., 2023; Piaulet-Ghorayeb et al., 2025; Radica et al., 2025), although mitigation efforts are underway (e.g., Rathcke et al., 2025). As a result of this contamination, in many cases the data are not sensitive to high mean molecular weight atmospheres that may be expected on these planets. Flares have proved to be a significant challenge to observations of the TRAPPIST-1 planets (Howard et al., 2023; Lim et al., 2023), with an estimated 3 flares per day large enough to impact transmission observations (Howard et al., 2023). While these stellar activity issues

challenge the analysis of current datasets, efforts are underway to remove contamination from both flares (Howard et al., 2023) and the transit light source effect (Allen et al., 2025; Rathcke et al., 2025).

Data reduction also introduces a source of uncertainty to final datasets, as different data reduction pipelines may yield different measurements and corresponding uncertainties. Additionally, in some cases the choice of underlying model to base reduction on may introduce bias (e.g., use of a sinusoidal model, forcing a particular ‘shape’, when fitting phase curve observations) (Gillon et al., 2026).

Modeling terrestrial planetary atmospheres presents the need for self-consistency, physical complexity, and statistical methods, balanced by the need for computational efficiency. In fitting models to observations of terrestrial planet atmospheres, highly detailed physical models must be conducted that account for geochemistry, photochemistry, climate processes, and radiative transfer for accurate spectral generation (e.g., Gialluca et al., 2026, In Review; Lincowski et al., 2023; Thomas et al., 2025). Using physically rigorous models allows us to make more informed interpretations of what planetary sources may be causing a particular signal, and provide information for follow up observations. Given the complexity of these processes, it is somewhat unsurprising that the majority of modeling challenges, attributed to the insufficient inclusion of physical processes, is caused by extreme computational expense. To self-consistently model the interplay between stellar radiation, planetary climate, and photochemistry, a coupled photochemical-climate model is used, but this approach requires extensive computation to find convergence for even a singular instance of the model. With very few observational datapoints, there are many degeneracies in fitting models to data, and so statistical sampling methods are often needed to fully understand the phase space of possible atmospheres. Fully self-consistent photochemical-climate models cannot be used in statistical approaches due to their computational expense. Instead, retrieval models are often used to flesh out the possible phase space, which rely generally on a radiative transfer solver to match likely spectral features to corresponding gas species, but this approach lacks knowledge of how molecules may interact in the atmosphere with each other or incoming radiation.

Following the complete loss of a primary atmosphere, it is not yet understood if geochemical outgassing can generate a secondary atmosphere, and maintain it against the intense stellar-driven atmospheric escape expected for M dwarf planets (Gialluca et al., 2021; Luger & Barnes, 2015). In general, models developed to match spectroscopic observations often fix atmospheric surface pressure and neglect realistic boundary conditions, using techniques like fixed mixing ratios to target a user-selected composition. However, by fixing surface pressure and/or omitting realistic boundary conditions, models cannot provide information on how the true sources and sinks of secondary atmospheres may equilibrate. In a common approach, mixing ratios of bulk constituents may be fixed at the top or bottom layer of the atmosphere, and the source and sink rates for that species are therefore inferred and updated to maintain this mixing ratio. By taking this approach, the outgassing and escape rates of gases are not set independently to be consistent with the geochemical and aeronomical knowledge (i.e., knowledge of upper atmospheric processes) of the planet. Furthermore, fixing the mixing ratio of certain species may neglect the actual source of that species in a realistic atmosphere. For example, if molecular oxygen (O_2) is fixed to be 80% at the surface of a lifeless world, the model will infer a direct flux of O_2 to maintain this mixing ratio,

but in reality abiotic O_2 is not typically produced in large quantities through direct volcanic outgassing, but rather through photochemical reactions often following the release of water or carbon dioxide. Thus, implicitly assuming O_2 is released directly in an atmosphere may miss the likely presence of other daughter products of species like water or carbon dioxide (e.g., OH , CO) (Catling, 2014; Meadows, 2017, e.g.). In a thick atmosphere, devoid of significant escape processes, this approach likely does not deviate from a model accounting for the balance of source and sink processes. However, the recent observations suggesting a thin atmosphere (if any) on the TRAPPIST-1 planets (e.g., Greene et al., 2023; Zieba et al., 2023) imply that a delicate balance of outgassing and escape is necessary to produce plausible tenuous atmospheric solutions. Therefore, research is needed that couples a physically complex atmospheric model, accounting for photochemistry and climate processes, to realistic boundary conditions (e.g., outgassing or escape fluxes) that allow the pressure of the atmosphere to evolve to an equilibrium.

5 Purpose & Structure of this Dissertation

In this dissertation, I develop a series of novel modeling approaches to simulate the generation and maintenance of tenuous secondary atmospheres on terrestrial exoplanets, directly demonstrating for the first time that plausible geochemical outgassing can create and sustain thin atmospheres against the intense expected stellar-driven escape from M dwarf hosts. Furthermore, I place a specific focus on constraining theoretical models with current observing campaigns made possible by JWST, ultimately taking a statistical approach that connects atmospheric boundary conditions, disequilibrium photochemistry, and spectroscopic observations. I focus specifically on one of the very first terrestrial exoplanet systems accessed through observation, TRAPPIST-1, though the techniques and conclusions of this body of work are broadly applicable to exoplanet characterization in the future. This work is extremely timely, in that it has been made possible for the first time by the recent flagship telescope, JWST (launched in winter 2021). Specifically, we conduct analyses on all aspects of TRAPPIST-1 planet evolution and explore a myriad of ways that computational models can be used in tandem with observation campaigns to teach us about the extant atmospheres in the system. This provides one of the earliest, most comprehensive analyses on a system of terrestrial exoplanets, and serves as pioneering work for efforts to understand other terrestrials in the future. We explore models for the evolution of radiative star-planet interactions; coupled photochemistry-climate processes; radiative transfer; and the use of geochemical and aeronomy models to inform atmospheric boundary conditions. Furthermore, we apply these tools in advanced computational frameworks, designed to work with super-computing resources, which often involve advanced statistical methods.

We begin by modeling hydrodynamic thermal atmospheric escape on all 7 planets driven by the host star’s PMS phase, informing likely water loss and subsequent abiotic O_2 production following planetary formation. This builds a foundation of knowledge for the likely histories of the planets, which can inform the expected atmospheres at present-day and suggest observational discriminants for the earliest observing campaigns. We then use this base knowledge to collaborate with geochemists and constrain the likely outgassing rates of key species (H_2O , CO_2) at present day (Thomas et al., 2025). With these outgassing rates,

and collaboration with experts in planetary aeronomy for balanced escape sinks, we conduct the largest sweep of self-consistent atmosphere modeling conducted yet for all TRAPPIST-1 planets, allowing the most likely regions of phase space to be guided by the combined data of all public observing campaigns at present (Espinoza et al., 2025; Glidden et al., 2025; Greene et al., 2023; Lim et al., 2023; Piaulet-Ghorayeb et al., 2025; Radica et al., 2025; Zieba et al., 2023). The massive amount of input combinations we are able to test in this sweep is made possible by the advanced automation of a coupled photochemical-climate modeling framework and the use of parallelization on HPC resources. Not only do we explore a vast number of present day atmospheres, we also remove historically used user constraints such as fixed species mixing ratios (forcing compositions) and fixed surface pressures. This shift allows our models to naturally find the surface pressure that balances the outgassing and escape processes, and the composition that results from our photochemical network.

In the final project we perform an in depth study of TRAPPIST-1c, one of the planets in the system with the most complete observational dataset. Using our modeling framework, plausible climate information, existing JWST observations, and techniques developed in the previous project, we use Bayesian nested sampling to determine plausible ranges for key planetary processes such as outgassing and escape for TRAPPIST-1c. This allows us to identify the most likely source and sink fluxes, atmospheric compositions, and pressures that match present-day observations, while folding in both model and observational uncertainty. This is one of the first attempts to fold in self-consistent photochemical modeling, advanced pressure-temperature profiles, and line-by-line radiative transfer into a retrieval-like framework meant to characterize the planetary environment in a statistically robust fashion.

Together, the projects in this thesis tell a story of the nature of planetary environments, from the interior through the atmosphere and into our telescope. In the next section (Chapter 2) we present all the methods used across the projects in this dissertation. We then provide specific chapters for each of the three projects contained here. An in depth discussion of the importance of this body of work together is given in Chapter 6. Finally, we conclude in Chapter 7.

CHAPTER 2

METHODS

Even the very wise cannot see all ends.

– J.R.R. Tolkien, “*The Lord of the Rings*”

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1 Modeling the Loss of Primordial Surface Volatiles

To explore the loss of a primordial water inventory and the loss of a primary steam and hydrogen atmosphere on the TRAPPIST-1 planets, we simulate the dominant process of hydrodynamic thermal atmospheric escape from the time of formation until either present-day, or the planet enters the habitable zone. We conduct our atmospheric loss simulations using VPlanet, an open source C-based code for modeling star, planet, and planetary system interactions and their impact on evolution (Barnes et al., 2020). VPlanet is broken up into modules for different physical processes; in this work, the STELLAR (stellar evolution, §1.1) and AtmEsc (atmospheric escape, §1.2) modules were used, and we specifically modify the treatment of diffusion-limited escape, the critical drag XUV flux, and the allowed behavior of the ratio of oxygen to hydrogen loss.

Input planetary and stellar parameters for our models come from Agol et al. (2021) and Birky et al. (2021), respectively. Using these updated constraints, we build and preserve self-consistent relationships between posteriors (see §1.3) allowing us to randomly sample a string of self-consistent planetary and stellar inputs for each simulation, as opposed to each input individually. Typically, 3500 – 5500 simulations are conducted per initial water content per planet to build distributions of final water and oxygen content. The exact number of simulations in a particular suite is determined by model convergence (found via the Kolmogorov–Smirnov, or K-S, test), which is described in Section 1.4. In Section 1.2.1, we illustrate the effects of our modifications to AtmEsc by comparing it to a simulation run with an older, validated version of the model (Lincowski et al., 2018, 2022; Luger & Barnes, 2015).

We note that a small number of outliers stemming from $\sim 1.24\%$ of the stellar mass samples were identified and removed from our distributions. These outlying stellar mass samples were greater than 4 standard deviations from the average and were likely a product of the machine learning method implemented in Birky et al. (2021). A more detailed description of outlier removal is given in Section 1.5.

1.1 Stellar Evolution (*STELLAR*)

The STELLAR module evolves the host star characteristics over time by performing a bicubic spline integration across mass and time of the evolutionary tracks in Baraffe et al. (2015) to track the stellar radius, radius of gyration, effective temperature, and luminosity from the PMS phase to present-day. It then uses the empirical broken power law formula of Ribas et al. (2005) to track the XUV output as a function of bolometric luminosity, which is particularly relevant for M dwarfs such as TRAPPIST-1:

$$\frac{L_{XUV}}{L_{Bol}} = \begin{cases} f_{sat} & \text{if } t \leq t_{sat}, \\ f_{sat} \left(\frac{t}{t_{sat}} \right)^{-\beta_{XUV}} & \text{if } t > t_{sat}, \end{cases} \quad (2.1)$$

where L_{XUV} is the XUV luminosity, L_{Bol} is the bolometric luminosity, t is the time, t_{sat} is the XUV saturation time, β_{XUV} is the exponential decay rate of the XUV luminosity, and

f_{sat} is the XUV saturation fraction, which is the ratio of XUV to bolometric luminosity during the saturation time; the latter 3 of these parameters are user defined inputs (see §1.3). The STELLAR module was used to fit the TRAPPIST-1 stellar input parameters that we use in this study (Birky et al., 2021; Fleming et al., 2020), and a more thorough and mathematical description of STELLAR can be found in Barnes et al. (2020); STELLAR was not modified in this work. The output stellar parameters from the STELLAR module become the input for the atmospheric escape model, AtmEsc, at each timestep; the stellar XUV characteristics, evolved by STELLAR, are the main driver of hydrodynamic thermal atmospheric escape.

1.2 Atmospheric Escape (*AtmEsc*)

Atmospheric escape can typically be split up into the thermal and non-thermal regimes; due to the heightened XUV environment, the TRAPPIST-1 planets are most likely subjected to primarily thermal escape processes during the PMS phase. For the innermost planets that never enter the habitable zone, thermal escape dominates throughout the lifetime of the atmosphere, but for the remaining planets, once the star reduces in luminosity sufficiently for them to enter the habitable zone, non-thermal escape processes have the potential to be more significant (e.g., Dong et al., 2018). Within the thermal regime we can consider Jeans escape or hydrodynamic blow-off – the latter occurring when the internal energy of the escaping species approaches the kinetic energy required for escape (Hunten, 1973); hydrodynamic loss is likely to provide a larger impact on the TRAPPIST-1 planetary atmospheres than Jeans escape, due to its extremely high mass loss rates.

Hydrodynamic escape can further be categorized as energy- or diffusion-limited. Energy-limited escape occurs when the escape flux is limited by the amount of energy incident on the planet, whereas diffusion-limited escape occurs when the escape flux is limited by the speed at which the escaping gas (typically hydrogen) can diffuse through a static background gas. During energy-limited escape, the escaping species may also drag a heavier species with it – the efficiency of which is highly dependent on mixing ratios in the atmosphere, the incoming XUV flux, and the mass of the species being dragged; thus, it can lead to observable effects such as mass fractionation of the heavier dragged species (e.g., Hunten et al., 1987; Zahnle et al., 1990), but this process produces only very weak fractionation of the hydrodynamically escaping species (i.e., D/H ratio, $^{18}\text{O}/^{16}\text{O}$) (Lammer et al., 2020; Mandt et al., 2009). This drag can also be a considerable source of atmospheric mass loss, particularly during a star’s most active period. In the diffusion-limited regime, the escape flux must be less than the maximum upward flux for which the background atmosphere is static (Hunten, 1973); thus, by definition, oxygen drag cannot occur under diffusion-limited escape. In the diffusion-limited regime mass fractionation may occur (Hunten et al., 1989; Zahnle et al., 1990), enhancing the atmosphere’s D/H ratio, but is likely only considerable on large timescales (Mandt et al., 2009).

We use VPLanet’s AtmEsc module to model both energy- and diffusion-limited escape for the TRAPPIST-1 planets; a full description of this module can be found in Barnes et al. (2020), but we provide a more succinct mathematical description of its implementation here. To start, the XUV environment determined by STELLAR serves as input to the atmospheric escape (AtmEsc) module of VPLanet (Barnes et al., 2020; Lincowski et al., 2018, 2022;

Luger & Barnes, 2015, and further updated in this work). In mathematically describing hydrodynamic escape, we begin by defining the reference hydrogen flux (F_H^{ref}), which is the flux of hydrogen off the planet in the absence of any other species. It is prudent to start with this quantity as the reference hydrogen flux is used as foundation for every possible mass loss flux off the planet. In this work we are considering only pure water atmospheres initially, therefore the reference hydrogen flux is in the absence of oxygen. Note, the reference hydrogen flux (given in $\text{atoms s}^{-1} \text{ cm}^{-2}$) is the true hydrogen flux for a planet in energy-limited escape and drag of a heavier species is shut off. Following Luger & Barnes (2015) and Schaefer et al. (2016), it is defined as:

$$F_H^{ref} = \frac{\epsilon_{XUV} F_{XUV} R_p}{4GM_p \mu} . \quad (2.2)$$

Here, ϵ_{XUV} is the XUV absorption efficiency, a fractional measure of the amount of incoming XUV flux that goes to driving escape; it is modelled following the treatment described in Bolmont et al. (2017), which calculated ϵ_{XUV} with a set of 1D radiation-hydrodynamic mass-loss simulations; we refer the reader to Figure 2 of Bolmont et al. (2017) for the range of adopted ϵ_{XUV} as a function of incoming XUV flux. F_{XUV} is the incoming XUV flux, R_p is the radius of the planet, M_p is the mass of the planet, and μ is the mass of one atomic mass unit (AMU).

After determining the reference hydrogen flux, the model will then determine if oxygen could be actively escaping via drag, the only oxygen sink directly modeled in this work. In energy-limited escape, drag occurs if the “crossover mass” (m_c) is greater than or equal to the mass of oxygen, and if the incoming XUV flux is greater than or equal to the critical drag XUV flux (F_{XUV}^{Crit}) (Hunten et al., 1987). Oxygen drag can also be shut off by the transition to diffusion-limited escape, but we will consider the aforementioned cases first. The crossover mass is the maximum particle mass that can be dragged by the escaping hydrogen flow; it is dependent on the reference hydrogen flux and, to fully describe the piecewise function of m_c , we first compare the reference hydrogen flux to an intermediary quantity, x (Luger & Barnes, 2015):

$$x = \left(\frac{m_O}{m_H} - 1 \right) (1 - X_O) \left(\frac{b_{diff} g \mu}{k_b T_{flow}} \right) . \quad (2.3)$$

Here m_O and m_H are the masses of an oxygen and hydrogen atom, respectively, X_O is the volume mixing ratio of oxygen, g is the surface gravity, T_{flow} is the temperature of the escaping flow, and b_{diff} is the binary diffusion coefficient for atomic oxygen being dragged by a hydrogen outflow, which is given in $[m^{-1} s^{-1}]$ by Zahnle (1986) as:

$$b_{diff} = 4.8 \times 10^{19} T_{flow}^{0.75} . \quad (2.4)$$

Note, as our atmospheres are solely composed of oxygen and water, $1 - X_O$ is equivalent to the volume mixing ratio of water (X_{H_2O}), which is a proxy for the mixing ratio of hydrogen.

With our quantity x in hand, we can define the crossover mass to be (Luger & Barnes, 2015):

$$m_c = \begin{cases} \mu + \frac{1}{1 - X_O} \frac{k_b T_{flow} F_H^{ref}}{b_{diff} g} & \text{if } F_H^{ref} < x, \\ \mu \times \frac{1 + \left(\frac{X_O}{1 - X_O} \right) \left(\frac{m_O}{m_H} \right)^2}{1 + \left(\frac{X_O}{1 - X_O} \right) \left(\frac{m_O}{m_H} \right)} + \frac{k_b T_{flow} F_H^{ref}}{\left(1 + X_O \left(\frac{m_O}{m_H} - 1 \right) \right) b_{diff} g} & \text{if } F_H^{ref} > x. \end{cases} \quad (2.5)$$

The other parameter that determines oxygen drag is the minimum incoming XUV flux required for drag to occur, known as the critical drag XUV flux, and is defined by (Schaefer et al., 2016):

$$F_{XUV}^{Crit} = \frac{4b_{diff}\nu_H^2}{\epsilon_{XUV}k_bT_{flow}R_p} \left(\frac{m_O}{m_H} - 1 \right) (1 - X_O), \quad (2.6)$$

where ν_H is the gravitational potential of hydrogen.

To summarize, oxygen drag will be shut off in the energy-limited regime if $F_{XUV} < F_{XUV}^{Crit}$ and/or $m_c < m_O$. If drag is occurring during energy-limited escape, the true hydrogen flux off the planet is less than the reference hydrogen flux and is given by:

$$F_H^{Drag} = F_H^{ref} \times \left(1 + \frac{X_O}{1 - X_O} \frac{m_O}{m_H} \frac{m_c - m_O}{m_c - m_H} \right)^{-1}. \quad (2.7)$$

While oxygen drag is occurring, we can define the flux of oxygen off the planet following Luger & Barnes (2015):

$$F_O = \frac{X_O}{1 - X_O} F_H \left(\frac{m_c - m_O}{m_c - m_H} \right) = \frac{\eta}{2} F_H. \quad (2.8)$$

Where η is defined as the ratio of oxygen escape to production:

$$\eta = \frac{2X_O}{1 - X_O} \frac{m_c - m_O}{m_c - m_H}. \quad (2.9)$$

Drag will also be halted in the diffusion-limited regime because it is defined when the background heavier gas is static, meaning the escape flux of hydrogen has been throttled sufficiently to prevent drag of a heavier species (Hunten, 1973). Following Schaefer et al. (2016), the switch to diffusion-limited escape occurs if the mixing ratio of free oxygen (i.e., oxygen not in water molecules) in the atmosphere is greater than or equal to the mixing ratio of water ($X_O \geq X_{H_2O}$). In this case, the true hydrogen flux off the planet again is less than the reference hydrogen flux and is given by (Luger & Barnes, 2015):

$$F_H^{Diff} = b_{Diff} g \mu \frac{\frac{m_O}{m_H} - 1}{k_b T_{flow} \left(1 + \frac{X_O}{1 - X_O} \right)}. \quad (2.10)$$

Now that we have defined all possible hydrogen flows off the planet, we can define the total water loss over time assuming the planetary radius is the effective XUV radius (Luger & Barnes, 2015):

$$\dot{M} = F_H 4\mu\pi R_p^2, \quad (2.11)$$

where F_H refers to whatever the true hydrogen flux is off the planet at a given time (e.g., F_H^{ref} , F_H^{Drag} , or F_H^{Diff}).

This further allows us to rewrite the oxygen flux off the planet during drag (equation 2.8) in terms of the water loss rate:

$$F_O = \frac{8 - 8\eta}{1 + 8\eta} \dot{M}. \quad (2.12)$$

In comparison to previous work with AtmEsc (Barnes et al., 2020; Lincowski et al., 2018, 2022; Luger & Barnes, 2015), we modify the treatment of the switch to diffusion-limited escape, implement a calculation of the critical drag XUV flux (Eq. 2.6), and change the allowed behavior of η (ratio of oxygen escape to production, Eq. 2.9) to be less restrictive; these changes follow Schaefer et al. (2016). In this work, the switch from energy- to diffusion-limited escape occurs when the mixing ratio of free oxygen (i.e., oxygen not contained in water molecules) is greater than or equal to the mixing ratio of water. The critical drag XUV flux (F_{XUV}^{Crit} , Eq. 2.6) is defined as the minimum incoming XUV flux required for oxygen drag to occur; if the incoming XUV flux is less than this, oxygen drag will be halted regardless of whether or not the escape is energy-limited. Finally, η is defined as the ratio of oxygen escape to production, or the ratio of oxygen to hydrogen loss. In past AtmEsc implementations, this was restricted to be ≤ 1 , meaning, at most, 1 oxygen atom could be lost for every 2 hydrogen atoms. Here, we allow η to vary up to ≤ 2 as we note that an accumulated oxygen reservoir may be depleted under highly favorable drag conditions, effectively meaning oxygen is lost faster than it is produced for certain periods of time. Future model improvements that could be made for a more realistic escape treatment are discussed during Chapter 3.

Our simulations make several assumptions, including initially pure water atmospheres, no surface oxygen sinks or geological activity, and that all water is on the planetary surface and available for escape by 1 Myr. As in Wordsworth et al. (2018), we assume no primordial H_2 -He envelope to be conservative in finding upper limit values of water loss and oxygen production. We explore initial water contents from 1 terrestrial ocean (TO) to 500 TO on a modified log space grid. We choose the upper limit for initial water content simulated here to be 500 TO, based on several recent studies which constrain the initial and present-day water mass fractions and suggest these are around 10%wt (e.g., Agol et al., 2021; Raymond et al., 2022; Schoonenberg et al., 2019), which would be equivalent to ~ 430 TO on a 1 Mearth planet; 500 TO is approximately bracketed between 10%wt of the larger planets, T1-b, c, and g, and the smaller planets, T1-d, e, f, and h. As we assume all oxygen not lost through escape remains in the atmosphere, our standard unit of measurement for oxygen production is bars of atmospheric pressure, which considers the mass and radius of a particular planet when converting from kg of oxygen. We additionally assume uniform mixing ratios for gases in the atmosphere (no vertical structure) with an isothermal temperature profile and do not consider photochemical processes besides the division of water molecules through photolysis.

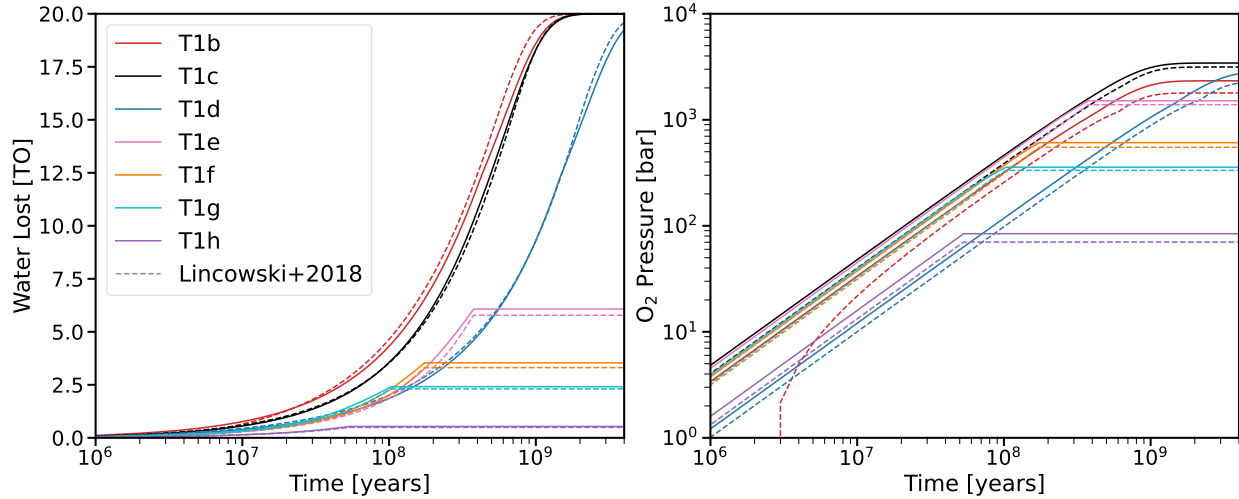


Figure 2.1: A comparison to the escape rates of the TRAPPIST-1 planets calculated in Lincowski et al. (2018, 2022) using constraints on the system from Grimm et al. (2018). **Left Plot:** The water lost in TO over time in years beginning with 20 TO initially. **Right Plot:** The oxygen produced in bars over time in years. Solid lines denote the rates calculated using the new version of AtmEsc from this work, and dashed lines denote the rates calculated using the version of AtmEsc from Lincowski et al. (2018, 2022).

1.2.1 Escape Model Validation

To show how the modifications to AtmEsc in this work have changed the outputs of the model from the original version (Barnes et al., 2020; Lincowski et al., 2018, 2022; Luger & Barnes, 2015), we present a comparison of one simulation from the original version of AtmEsc to the version modified in this work. Figure 2.1 shows an escape rate calculation for a single simulation of the TRAPPIST-1 planets with an initial water content of 20 TO from Lincowski et al. (2018, 2022), compared to the same calculation done with our model upgrades using the same input parameters. Note, as Lincowski et al. (2018, 2022) used inputs for the TRAPPIST-1 system defined by Grimm et al. (2018), this comparison is meant to show the differences in the models and does not use the updated constraints on the system we adopt in the rest of our work. Additionally, we adopt the same XUV model in this calculation as Lincowski et al. (2018, 2022).

There are only minor differences between the two versions of AtmEsc in our comparison. In both models T1-b and c become desiccated, and T1-d is nearly desiccated, losing ~ 0.14 TO more water in Lincowski et al. (2018, 2022). The three interior planets all produce $\sim 10 - 30\%$ more oxygen in this work; this is because Lincowski et al. (2018, 2022) predicts faster desiccation on these planets, meaning oxygen drag is more efficient during periods of greater water loss preventing build-up. The outer planets all lose more water in this work, typically by ≤ 0.2 TO, and as a result build up more oxygen, typically by ≤ 100 bars.

1.3 VPlanet Input Description

In determining VPlanet simulation inputs, we consider not only observational uncertainty in the stellar luminosity evolution and physical planetary parameters (Agol et al., 2021; Birky et al., 2021), but also that planetary parameters such as mass, radius, orbit and insolation can be self-consistently dependent on the assumed stellar environment, as planetary mass and radius are derived from planet-to-star ratios. To account for this, we construct self-consistent chains of input parameters for the entire system, such that one simulation randomly samples an input chain as opposed to each individual parameter separately.

Here we detail the stellar and planetary parameters we consider, and how the input chain construction for a single simulation is accomplished, which is then repeated for simulation suites at a particular initial water content. The stellar inputs used in our work (from Birky et al., 2021) are the mass of the star (M_*), the XUV saturation fraction (f_{sat}), the XUV saturation time (t_{sat}), the exponential decay rate of the XUV luminosity (β_{XUV}), and the age (τ). For each of the 7 planets, the input parameters used (from Agol et al., 2021) are the planetary mass ratio (M_p/M_*), the planetary radius ratio (R_p/R_*), the eccentricity (e), and the orbital period (P). More specifically, Agol et al. (2021) presents a transit timing and photodynamical analysis of the system; the former, transit timing variations (TTV), are highly sensitive to the ratios of planetary to stellar mass, along with the eccentricity and orbital period. The photodynamical analysis provides sensitive constraints on the stellar density (ρ_*) and planet-to-star radius ratios by combining the mass ratios and orbital parameters derived from the TTV analysis to improve the derivation of planetary and stellar densities from Spitzer photometry (Agol et al., 2021). Thus, the actual planetary mass and radius of a single input chain will be dependent on the sampled stellar parameters.

To construct one input chain, one suite of stellar, TTV, and photodynamical inputs are randomly sampled. The selected stellar mass is then combined with the stellar-to-planetary mass ratios from the TTV sample to produce the planetary masses:

$$M_{p,i} = \frac{M_{p,i}}{M_*} M_* , \quad (2.13)$$

where i refers to the planet in question (b, c, d, e, f, g, or h). Using Eq. (2.13) to find the planetary mass creates a relationship between the stellar inputs and the TTV inputs. The same stellar mass is then used to find the stellar radius using the stellar density from the photodynamical inputs (Agol et al., 2021):

$$R_* = \left(\frac{3M_*}{4\pi\rho_*} \right)^{\frac{1}{3}} . \quad (2.14)$$

Finally we can take this stellar radius and combine it with our stellar-to-planetary radii ratios to get the planetary radii:

$$R_{p,i} = \frac{R_{p,i}}{R_*} R_* . \quad (2.15)$$

Thus, by using one sampled stellar mass and Equations (2.13) through (2.15), a self-consistent relationship between all priors is built. For our constructed set of input chains, no single stellar, TTV, or photodynamical sample from Birky et al. (2021) and Agol et al.

(2021) is used more than once; and likewise, no one input chain is used more than once in a given simulation suite (i.e., at a given initial water content).

The process of sampling input chains is facilitated by VSPACE (Barnes et al., 2020), an open source support routine for VPLANET that creates a suite of input files for the model across a parameter space defined by the user; sampling from user-defined input distributions is new functionality that has been added to VSPACE in this work. Finally, Tables 2.1 and 2.2 show the 50th percentile values and 1- σ uncertainties of the system’s physical parameters, found from 20,900 input chains using the probability distributions described in Agol et al. (2021) and Birky et al. (2021). Since we fold in uncertainty in the stellar mass reported by Birky et al. (2021), our planetary mass and radii uncertainties reported in Table 2.1 may differ slightly than those reported in Agol et al. (2021), despite using identical mass and radius ratios, because they sampled stellar mass from $0.09016 \pm 0.001 M_{\odot}$.

Body	Mass [$M_{\oplus}$]	Radius [$R_{\oplus}$]	Eccentricity	Orbital Period [Days]
T1-b	$1.377^{+0.063}_{-0.062}$	$1.117^{+0.009}_{-0.007}$	$0.00401^{+0.00266}_{-0.00233}$	$1.510826^{+0.000005}_{-0.000005}$
T1-c	$1.311^{+0.044}_{-0.045}$	$1.098^{+0.010}_{-0.008}$	$0.00190^{+0.00192}_{-0.00133}$	$2.421936^{+0.000017}_{-0.000017}$
T1-d	$0.388^{+0.008}_{-0.008}$	$0.789^{+0.009}_{-0.008}$	$0.00583^{+0.00129}_{-0.00141}$	$4.049219^{+0.000026}_{-0.000025}$
T1-e	$0.693^{+0.013}_{-0.014}$	$0.922^{+0.010}_{-0.009}$	$0.00637^{+0.00103}_{-0.00080}$	$6.101013^{+0.000035}_{-0.000034}$
T1-f	$1.040^{+0.017}_{-0.017}$	$1.046^{+0.010}_{-0.009}$	$0.00848^{+0.00103}_{-0.00118}$	$9.207540^{+0.000030}_{-0.000029}$
T1-g	$1.322^{+0.019}_{-0.019}$	$1.131^{+0.011}_{-0.009}$	$0.00404^{+0.00101}_{-0.00091}$	$12.352445^{+0.000054}_{-0.000052}$
T1-h	$0.325^{+0.019}_{-0.018}$	$0.756^{+0.012}_{-0.012}$	$0.00370^{+0.00068}_{-0.00072}$	$18.772868^{+0.000217}_{-0.000209}$

Table 2.1: 50th percentile values for all planetary parameters used as input found from 20900 samples. Uncertainties given are set by 16th and 84th percentile values (1 σ). Values come from transit timing and photodynamical analysis in Agol et al. (2021) combined with stellar mass from Birky et al. (2021).

1.4 VPLANET Convergence

To create probability distributions of the final water loss and oxygen production on each planet per initial water content, we systematically add simulation outcomes to a distribution until convergence is achieved, i.e., when the addition of simulations to the sample no longer changes the 3 σ confidence intervals of the resulting distribution. This process begins with an initial set of 500 simulations, whose final water and oxygen mass comprise the initial distribution of escape outcomes. A step is then taken, defined as the addition of 100 simulation outcomes to the distribution. The difference between the probability distributions from before and after the step is then quantified by the two-sample K-S test, which essentially determines how likely it is that the two distributions originated from the same (unknown) parent distribution. This process of taking steps is continued until the K-S statistic is 0.0004 or less, which we empirically determined to be converged, meaning the addition of more

Parameter	Value
Mass [$M_{\odot}$]	$0.090^{+0.001}_{-0.001}$
XUV Saturation Fraction [$\log_{10}(L_{XUV}/L_{Bol})$]	$-3.030^{+0.251}_{-0.231}$
XUV Saturation Time [Gyr]	$3.146^{+2.217}_{-1.459}$
XUV Decay Rate	$-1.172^{+0.270}_{-0.277}$
Age [Gyr]	$7.962^{+1.783}_{-1.867}$

Table 2.2: 50th percentile values for all stellar parameters used as input found from 20900 samples. Uncertainties given are set by 16th and 84th percentile values (1σ). Values come from Birky et al. (2021).

simulations no longer appreciably changes the results. As an added precaution, the model is required to report convergence for 3 consecutive steps before it declares global convergence has been achieved and the result finalized. Typically this process requires approximately 3500 – 5500 simulations per planet per initial water content.

This process is facilitated by Vconverge, an open source support routine for VPLanet (Barnes et al., 2020) that has been created for this work. Vconverge uses the updates made to VSPACE (described in the previous Section 1.3) to create the input files needed for the initial simulation set, and each subsequent step of 100 simulations. This support routine then automates the process described in this section to find convergence.

We run simulation suites over a modified log grid of initial water contents spanning 1 – 500 TO. From 1 – 20 TO, we use a step size of 1 TO; from 20 – 100 TO, we use a step size of 10 TO; then from 100 – 500 TO, we use a step size of 100 TO. In total, 32 initial water contents are considered. In the case of T1-e, an additional 9 simulation suites were run between 100 – 200 TO, with a step size of 10 TO, to achieve the results shown in Section 3.3.1. These additional simulation suites are only considered with respect to that result, as their inclusion would not affect any other paper result.

1.5 VPLanet Outlier Removal

Within our full dataset across all initial water contents, a small subset of simulations were identified as outliers originating from the stellar mass samples. As discussed in Section 1.3, we sample stellar and planetary inputs from Birky et al. (2021) and Agol et al. (2021), respectively, creating 20,900 input strings a simulation could draw from. Figure 2.2 shows the stellar mass samples plotted on the y-axis, with an arbitrarily assigned ID number on the x-axis. The majority of samples fall within 2 standard deviations from the mean, but a small group of samples lie at stellar masses greater than 4 standard deviations from the mean, which we adopt as our outlier cut-off. Outliers account for 259/20900, or 1.24%, of all samples. Simulations using a stellar mass above this cut-off are removed from the final dataset.

These outliers originate from the process used in Birky et al. (2021) to fit the stellar mass

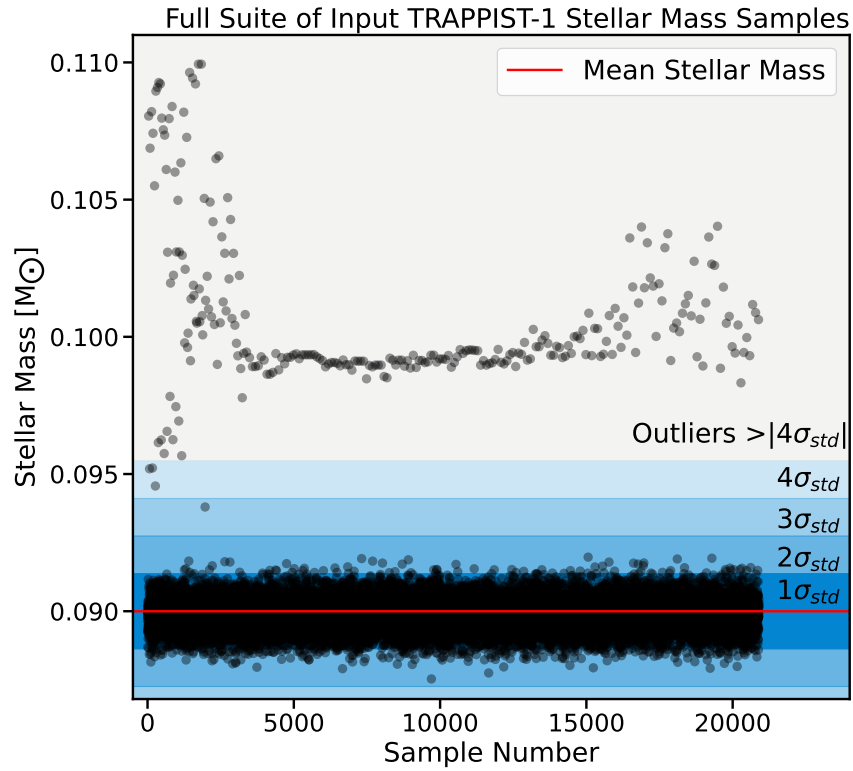


Figure 2.2: All 20,900 stellar mass samples available for simulations to draw from (from Birky et al., 2021). The y-axis shows the stellar mass in $M_{\odot}$ of a given sample, which are arbitrarily assigned an ID on the x-axis. The red solid line denotes the mean stellar mass across all samples, while the dark blue and subsequent lighter blue regions denote 1, 2, 3, and 4 standard deviations from the mean, as labeled in the plot. The light grey shaded region denotes samples greater than 4 standard deviations from the mean, indicating that samples in this region are classified as outliers, such that simulations using stellar masses above 4 standard deviations are removed from the final data set.

of TRAPPIST-1 with the most recent observational data. They used a Gaussian process (GP) surrogate model to estimate the probability of an input parameter, including stellar mass, given the observed stellar properties. Sampling of the GP surrogate posterior was performed using the emcee package (Foreman-Mackey et al., 2013). We found that these outliers originated from the randomized initial state of the MCMC walkers, suggesting that number of burn-in samples reported in the posterior samples by Birky et al. (2021) was insufficient. The burn-in period was taken to be 2x the average autocorrelation time, which appeared to not reflect the converged state for a subsample of the MCMC walkers. Thus, these outlying stellar mass samples are likely a product of randomized initial walker states, and as they account for 1.24% of all samples, we conclude their removal is justified.

2 Coupled Photochemical-Climate Model Framework

Chapters 4 and 5 use photochemical, climate, and radiative transfer models in coupled frameworks to generate a terrestrial secondary atmospheres balanced by interior outgassing, surface deposition, and top-of-atmosphere (TOA) escape. We use a variety of component models coupled together that consider photochemistry, climate, radiative transfer, changing surface pressure adjustments, and geochemical outgassing; each of the component models called in our broader coupled frameworks is described in §2.1. We first discuss a forward model pipeline that is fully self-consistent, coupling photochemistry to climate calculations, in §2.2. This fully self-consistent pipeline is used to complete grid sweep simulation suites across a broad phase space, which is presented in Chapter 4 and Gialluca et al. (2026, In Review). Following our grid sweep analyses, we transition to a Bayesian statistical inference modeling framework that targets likely atmospheric boundary conditions for the interior planet T-1c, whose forward modeling strategy applies modifications of our fully self-consistent pipeline; the statistical inference forward model pipeline and Bayesian inference sampling strategy is described in §2.3. Finally, we describe the atmospheric inputs and boundary conditions used in both our grid sweep and statistical inference analyses in §2.4.

The particular component models, we employ are the *Atmos* photochemical model (§2.1.1; Arney et al., 2016; Lincowski et al., 2018; Meadows et al., 2018a), the Line-By-Line Absorption Coefficients model (*LBLABC*; Meadows & Crisp, 1996), the Spectral Mapping Atmospheric Radiative Transfer Tool (*SMART*, §2.1.2; Crisp, 1997; Meadows & Crisp, 1996), and the *VPL Climate* model (§2.1.3; Lincowski et al., 2018; Meadows et al., 2023; Robinson & Crisp, 2018). In this body of work, we additionally develop a novel routine to allow the surface pressure of a modeled atmosphere to vary, which is called following a photochemical model run; this surface pressure adjustment is described in §2.1.4. Outgassing rates used as inputs in our simulations are constrained by the model of Thomas et al. (2025), described in §2.1.5. Across our modeling pipeline, we use the Peacock et al. (2019) stellar spectrum of TRAPPIST-1, which is visualized in Figure 2 of Meadows et al. (2023).

These models are first called by a python wrapper developed in this dissertation to iterate self-consistent atmospheres to convergence — considering fully coupled photochemical-climate calculations — enabling the exploration of a broad range of input boundary conditions for all seven TRAPPIST-1 planets (§2.2); this phase space exploration corresponds to the research of Chapter 4. Then, we build a Bayesian statistical inference framework (via the

MultiNest algorithm, Buchner et al., 2014; Feroz et al., 2009) to constrain input atmospheric boundary conditions for a photochemical model of T-1c that best generate atmospheres reproducing the available emission data (Gillon et al., 2026; Zieba et al., 2023); this statistical exploration corresponds to the research of Chapter 5.

We improve on past work by massively parallelizing atmosphere generation on HPC resources to explore a wide range of boundary conditions, and we add a routine to automatically update surface pressure in response to outgassing and escape. We consider atmospheres sustained by H₂O and/or CO₂ outgassing, and we further consider the addition of trace SO₂ (up to 1%) at the surface level.

2.1 Component Models

2.1.1 The Atmos Photochemical Model

The *Atmos* photochemical model (Arney et al., 2016; Kasting et al., 1979) self-consistently accounts for the effects of incident radiation on atmospheric composition. Of particular relevance to the present study, Lincowski et al. (2018) updated *Atmos* to treat M dwarf hosts more realistically by including new cross sections and a higher resolution sampling grid in the UV; this update includes an extended H₂O cross section, which may be critical for H₂O photolysis when shielded by other species (Ranjan et al., 2020). *Atmos* has already been used in several studies to model both anoxic and extremely oxidized atmospheres in the TRAPPIST-1 system (e.g., Lincowski et al., 2018, 2023; Meadows et al., 2023; Zieba et al., 2023). In depth descriptions of *Atmos* can be found in Arney et al. (2016); Lincowski et al. (2018); Meadows et al. (2018a), but we provide a basic description here.

For a given model, species and reaction lists are specified to *Atmos*, which applies a vertical transport scheme (including molecular and eddy diffusion) to the atmosphere divided into 200 plane parallel layers assumed to be in hydrostatic equilibrium. There are 251 chemical reactions in our network, 49 of which are photolysis reactions. We include 59 long-lived species, 7 short-lived species (calculated in equilibrium at each timestep), and 1 inert gas (N₂); all species are composed of hydrogen, oxygen, carbon, nitrogen, and/or sulfur. Our chemical reaction network was created by adopting the H₂O, O₂, CO₂, and SO₂ reaction networks presented by Lincowski et al. (2018) for TRAPPIST-1 and Venus models (used also by Lincowski et al., 2023, for TRAPPIST-1c). In *Atmos*, surface boundary conditions for a given species can be set as a constant mixing ratio, a constant outgassing flux, or a surface deposition velocity. Top of atmosphere boundary conditions may be given as a constant escape flux or an effusion velocity; for Hydrogen specifically, diffusion-limited escape rates are calculated automatically.

In this work, we set boundary conditions as constant fluxes or deposition/effusion velocities based on literature constraints and allow the model to determine the resulting surface pressure that arises from the balance of sources and sinks in a given simulation. As we are interested in determining if thin atmospheres can be sustained by outgassing alone, a novel approach used in this work is to treat the surface pressure as a dependent variable, rather than fixing it in a given atmosphere. Note, unlike all other gases considered in this work, we do consider a trace fixed amount of SO₂ in certain experiments. However, this mixing ratio never exceeds 1% and does not significantly constrain the equilibration of the atmospheric

pressure under the influence of outgassing, escape, and photochemistry.

2.1.2 Radiative Transfer Modeling: SMART & LBLABC

We generate spectra with the Spectral Mapping Atmospheric Radiative Transfer (*SMART*) model, a 1D line-by-line, multistream, fully multiple scattering radiative transfer model (Crisp, 1997; Meadows & Crisp, 1996; Robinson, 2017) that has been validated against the observed spectra of several solar system bodies including Earth (Robinson et al., 2011), Mars (Tinetti et al., 2005), Titan (Robinson et al., 2014), and Venus (Arney et al., 2014; Lincowski et al., 2021). *SMART* adopts the line-by-line radiative transfer solver DISORT (Stamnes et al., 1988, 2000). Furthermore, *SMART* has been used to model the preindustrial and Archean Earth (e.g., Arney et al., 2016; Currie et al., 2023) and it has been used extensively to model a variety of atmospheres in the TRAPPIST-1 system (Gialluca et al., 2021, 2023; Lincowski et al., 2018, 2023; Lustig-Yaeger et al., 2019a; Meadows et al., 2023; Zieba et al., 2023). At a specified wavelength range and resolution, *SMART* can generate planetary spectra given a pressure-temperature profile, gas mixing ratios, UV-visible and collisionally induced absorption cross sections, absorption coefficients generated by the Line-By-Line ABsorption Coefficients (*LBLABC*) model (Meadows et al., 2018a) using the HITRAN line database (Gordon et al., 2022), a stellar spectrum, and wavelength-dependent surface albedo. In this work we neglect clouds and hazes.

2.1.3 The VPL Climate Model

The *VPL Climate* Model is a terrestrial radiative-convective equilibrium climate model that can either be used in 1D or 1.5D (two column day-night sides) (Lincowski et al., 2018, 2023; Robinson & Crisp, 2018). This climate model is based on the previously described SMART radiative transfer model (Meadows & Crisp, 1996). *VPL Climate* uses time stepping to advance the temperature profile of an atmosphere towards equilibrium, defined by the 1D surface-atmosphere thermodynamic energy equation. Heating rates are determined via the Linearized Flux Evolution method (LiFE, Robinson & Crisp, 2018), which uses spectrally resolved Jacobians generated by SMART to calculate changes in radiative fluxes in response to changes in temperature. Whenever atmospheric properties evolve outside of the linear range of Jacobians, they are recalculated by SMART. Furthermore, mixing length theory is used to calculate convective heat fluxes and heating rates (treatment fully described in Lincowski et al., 2018, with updates by Meadows et al., 2023).

The 1.5D, or two column, mode of *VPL Climate* is used to generate profiles for the day and night sides of a terrestrial planet; the methods of this mode are described by Lincowski et al. (2023). The 1.5D mode of *VPL Climate* additionally calculates day-night heat transport through horizontal winds. This 1D version of *VPL Climate* has been validated against 3D GCMs (Meadows et al., 2018a) and more critically, Earth and Venus profiles (Lincowski et al., 2018; Meadows et al., 2023), and the two-column mode has been validated against GCM-generated phase curves (Lincowski et al., 2018, 2023). Both the 1D and two column version of *VPL Climate* have also been used specifically to model planets in the TRAPPIST-1 system (e.g., Lincowski et al., 2023; Meadows et al., 2023). In this work, the two column mode is used only for the interior planets of the TRAPPIST-1 system (b, c, and d) which

may have dayside emission data in hand or are hot enough for it to be feasibly collected in the future.

2.1.4 Surface Pressure Adjustment Routine

To identify atmospheres which are the equilibrium state between outgassing and vigorous escape on these planets, a novel routine is developed in this work to update the surface pressure of a given atmosphere simulation while trying to find convergence between the photochemical and climate models. During one modeling pass through *Atmos*, the pressure and number density of each model layer is fixed. Because of this, although mass is conserved in the atmosphere, the total mixing ratio of a layer (sum of mixing ratios for all species) may depart from 1. For example, if a layer begins with a number density of 1 cm^{-3} and only contains 1 O_2 molecule, the total mixing ratio, equal to the mixing ratio of O_2 , would be 1. If this O_2 molecule was then photolyzed to 2 O atoms, the number density of the layer would remain fixed and therefore the total mixing ratio, now equal to the mixing ratio of atomic O, would be 2. In other words, if the cumulative atmospheric sources provide more or insufficient material needed for the set pressure, the total mixing ratio of all gases may indicate this by being greater than or less than 1. In many past studies, focused on matching best-fit models to observations (e.g., [Lincowski et al., 2023](#)), boundary conditions have been set by fixed mixing ratios, which allow the model to then infer the required outgassing or loss flux to maintain a total mixing ratio near 1 for a chosen pressure. We improve on past work by moving away from fixed mixing ratio boundary conditions to allow the surface pressure of the atmosphere to equilibrate based on input fluxes that have been identified in the literature as realistic for the TRAPPIST-1 planets (see §2.4). We leverage this new functionality to test if thin atmospheres, which are still consistent with JWST observations ([Ducrot et al., 2025](#); [Greene et al., 2023](#); [Ih et al., 2023](#); [Lim et al., 2023](#); [Lincowski et al., 2023](#); [Radica et al., 2025](#); [Zieba et al., 2023](#)), are also theoretically plausible from realistic outgassing.

As noted above, *Atmos* adopts a fixed pressure or number density versus altitude profile during a single model iteration. To automatically adjust the surface pressure of a given atmosphere between iterations of *Atmos*, we calculate a corrected number density profile by scaling the fixed number density profile reported by the previous model run by the total mixing ratio (sum of all species mixing ratios), which acts as a renormalization factor. This corrected number density profile is integrated over altitude to find a column density, and subsequently a column mass, from which a revised surface pressure is derived. The pipeline will iterate between running *Atmos* and updating its surface pressure until the surface pressure is changing by less than some tolerance, $<3\%$ for grid sweep analyses and $<5\%$ for statistical inference analyses.

When adjusting the surface pressure, we first find the corrected total number density per atmospheric layer from the reported number density and volume mixing ratios (which may be greater or less than 1):

$$n_{\text{corr},z} = n_{\text{report},z} \sum_i X_{i,z} . \quad (2.16)$$

Here, for a given altitude layer z , the number density reported by the previous model run ($n_{\text{report},z}$) is scaled by the total mixing ratio of that layer (the sum of all i species mixing ratios, $X_{i,z}$) — this provides the corrected number density for that layer, $n_{\text{corr},z}$. We then

find the column number density by integrating the corrected number density profile over altitude:

$$N_{col} = \int_z^\infty n_{corr,z} dz . \quad (2.17)$$

Note, we complete integration in the model using *Numpy*'s trapezoidal integration scheme (Harris et al., 2020a). The column number density can be converted to the column mass using the atmospheric mean molecular weight, μ , and Avogadro's number, N_{Avo} :

$$\sigma_{col} = \frac{N_{col} \mu 10^{-3}}{N_{Avo}} , \quad (2.18)$$

assuming μ is in the units of g/mol and N_{col} is in the units of m^{-2} , the factor of 10^{-3} converts the column mass to units of kg/m^2 . Finally, the corrected surface pressure can be found with the column mass and the planetary gravity, g :

$$P_{surf,corr} = \sigma_{col} g . \quad (2.19)$$

After creating an atmosphere model with *Atmos*, this routine can calculate the corrected surface pressure (Eq. 2.19) and rerun *Atmos*, if necessary.

2.1.5 Input Volatile Outgassing Model

Although present data on the TRAPPIST-1 planets does not provide direct constraints on geologic properties or outgassing, the volatile outgassing rates used as input in this study are taken from Thomas et al. (2025), who place theoretical boundaries on these quantities consistent with observations of the system (e.g., Agol et al., 2021) and knowledge of solar system bodies. While the densities of the planets are known to within 5% accuracy (Agol et al., 2021), the space of possible interior compositions and structures consistent with these observed densities is highly degenerate (e.g., Agol et al., 2021; Elkins-Tanton & Seager, 2008). Other key information related to volatile outgassing is similarly unconstrained, such as the magma emplacement rate and bulk mantle volatile abundances. Given these uncertainties, the true interior structures, and related outgassing rates, for the TRAPPIST-1 planets are unknown.

Thomas et al. (2025) placed theoretical bounds on the TRAPPIST-1 outgassing rates by statistically exploring a broad range of interior scenarios spanning the full range of conditions that are theoretically possible on terrestrial planets and empirically observed in the solar system (on Earth, Mars, Venus, and Io). First, the model samples the mantle water content from negligible values (0.01 wt%) up to the maximum value a terrestrial planet can sustain without becoming thermodynamically unstable (~ 1 wt%, according to Guimond et al., 2023). Next, the amount of water partitioned into the magma is calculated, limited by either the water abundance or solubility, both of which are calculated under the range of physical conditions observed during the production of Earth's mantle-derived magmas (Sigurdsson et al., 2015). The magma emplacement rate, which is the most uncertain, is either sampled from thermal evolution models of TRAPPIST-1 ($0.01 - 8500 \text{ km}^3 \text{ yr}^{-1}$; Krissansen-Totton & Fortney, 2022) which span from negligible to an order of magnitude higher than Io, or it is fixed at values measured for Earth, Mars, and Io. In the present study, however, we restrict

our analysis to samples that adopt magma emplacement rates derived from the TRAPPIST-1 thermal evolution models. Equilibrium degassing from the emplaced magma is calculated under the range of chemical conditions observed in the solar system (e.g., magma oxygen fugacity ranging defined by FMQ-4 to FMQ+4, magma temperature ranging from 873 K to 1973 K, etc). Finally, additional filters are applied to incorporate empirical information on the TRAPPIST-1 system, such as strong observational constraints that preclude large H₂-dominated atmospheres (De Wit et al., 2018; Wakeford et al., 2019) implying that H₂ cannot be the most abundant outgassed species.

Given the broad phase space and uncertainties considered, the Thomas et al. (2025) outgassing rates vary widely. For example, when all parameters are sampled over their full ranges, the water outgassing rate on T-1c can span ~ 6 orders of magnitude. Therefore, we sample from these distributions in our modeling approach by initially testing the 2.5th, 50th, and 97.5th percentile values (median and lower/upper 2 σ) of the Thomas et al. (2025) outgassing rate distributions for all 7 planets.

2.2 Fully Self-Consistent Forward Modeling

We first develop a python framework which takes a novel approach to coupling *Atmos*, *VPL climate*, *LBLABC*, and *SMART* by automating a single atmosphere model run to convergence and parallelizing multiple models within an input phase space of atmospheric source and sink rates. We employ nested local convergence checks to determine global convergence across three stages: photochemical modeling, surface pressure adjustment, and climate modeling. The wrapper begins by iteratively running the *Atmos* photochemical model, with an initial state and selected boundary conditions, until it reaches local photochemical convergence. Local convergence of the photochemical model is dependent on both the final timestep size, and on the change in gas abundances across a run. Since *Atmos* uses a variable timestepping method, the size of the timestep increases as the atmosphere approaches equilibrium and the rates of change in gas abundances decrease. Once the timestep has reached 10¹⁷ seconds (>3 Gyr), indicating the atmosphere has achieved stability over long timescales, the first *Atmos* convergence criterion is met. The other criterion we employ for iterated local convergence of *Atmos* requires that the summed fractional changes in abundance for all absorbers present at $\geq 0.1\%$ remains less than 1, thereby testing the stability of primary constituents from the beginning to the end of the model run. When both the timestepping criterion (must be $>10^{17}$ seconds) and the cumulative fractional abundance change criterion are met, local *Atmos* convergence is achieved.

After *Atmos* finds convergence, the surface pressure is adjusted, and *Atmos* is run to local photochemical convergence again. This process of iterating between the surface pressure adjustment and *Atmos* is repeated until the surface pressure changes by less than 3% following the convergence of *Atmos*. Once the surface pressure is stable, line-by-line absorption coefficients are created with *LBLABC* and passed to the *VPL Climate* model, which is iteratively run to local climate convergence. Local convergence of the climate model occurs when the heating rate in the troposphere is less than 0.09 K/day, and all atmospheric layers are flux balanced within 1 W/m². After local climate convergence is achieved, the resulting temperature profile is passed back to *Atmos*, and the process restarts.

When transitioning from the photochemical to the climate portion of the pipeline, *VPL*

Climate receives the gas abundance profiles for the most radiatively active species previously calculated by *Atmos*. The climate model then updates the temperature profile and the eddy diffusion rates, which are passed back to the photochemical model for the next iteration of the pipeline. In summary, the photochemical model updates gas abundance profiles and the climate model updates temperature and eddy diffusion profiles; these quantities are exchanged between the two models as the pipeline iterates towards global convergence. This method of iterating photochemical and climate models separately is commonly used for modeling planetary atmospheres (e.g., Agúndez, 2025; Arney et al., 2016; Lincowski et al., 2023).

Global convergence checks occur after the surface pressure adjustment process once a full loop is completed (i.e., photochemical modeling through climate modeling with local convergence). Global convergence is achieved when, on a single pass through all modeling stages, the climate model finds local convergence on the first attempt, and the surface pressure never changes by more than 3%. A flowchart illustrating this iterative photochemical-climate modeling process is shown in Figure 2.3.

Once global convergence is achieved in the coupled photochemical-climate portion of the modeling framework, transmission spectra are generated for the terminator portion of the planet (i.e., global average). In the case of planets that possess emission data (T-1b and c) or planets that may be reasonably accessible in the future with emission observations (T-1d), we further calculate day-night climate profiles and generate emission spectra. To produce the day and night side temperature profiles, the *VPL Climate* model is used in 2 column mode and must find convergence where all atmospheric layers are flux balanced within 1 W/m² for *both* the day and night side profiles. If 2 column convergence cannot be found, the atmosphere is rejected from being a possible solution. With the day and night profiles, transmission and emission spectra are then generated by SMART.

2.2.1 Grid Sweep Exploration Strategy

When conducting the initial atmospheric source and sink phase space exploration (Chapter 4), we organize our exploration of the parameter space into three phases. In the first phase, we focus on atmospheres that are fueled only by water outgassing, and are depleted in carbon or sulfur bearing species. This phase begins with an initial simulation suite that is standardized for all planets (inputs ranges described and justified in §2.4) which includes H₂O outgassing, O₃ and H₂O₂ dry deposition, and H₂, H, O, and O₂ TOA loss. The initial simulation suite contains 64 simulations per planet, though many of these simulations may ultimately not be viable. Based on the results of the initial simulation suite, we vary specific sources and sinks to push the model towards stable, converged atmospheres.

The second phase of our exploration repeats this process considering a combination of both H₂O and CO₂ outgassing. In addition to the sinks previously described in the H₂O outgassing only phase, we also consider CO dry deposition and CO₂ TOA escape. At the end of both the first (H₂O outgassed) and second (H₂O-CO₂ outgassed) phase of exploration, we compile all stable atmospheres across all simulation suites and test the addition of trace SO₂. Trace SO₂ is added as a fixed mixing ratio of 100 ppm, 0.1%, or 1% at the surface, so the balance of SO₂ source to sink is automatically adjusted in the bottom layer to maintain the set trace mixing ratio. Above the surface layer, SO₂ is subject to the standard photochemical

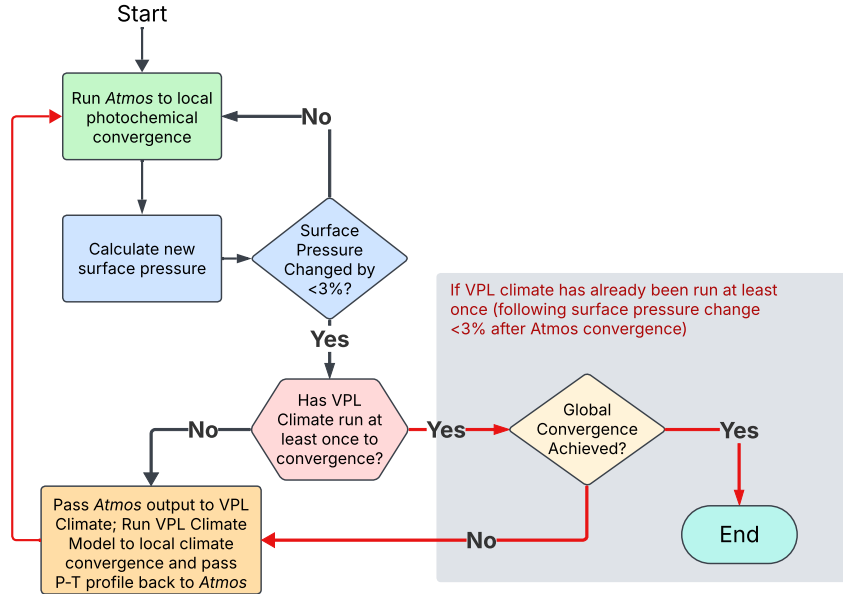


Figure 2.3: Flowchart describing how a single atmosphere model is run to convergence through the coupled photochemical-climate modeling. This is described in §2.2.

model, i.e., the mixing ratio is not fixed or constrained at any other layer.

2.3 Statistical Inference Forward Modeling

Following the application of our fully self-consistent forward model pipeline described above and applied in Chapter 4, we turn to Bayesian inference to statistically constrain input atmospheric boundary conditions for a photochemical model of T-1c that best generate atmospheres reproducing the available emission data (Gillon et al., 2026; Zieba et al., 2023). We select T-1c specifically as the subject of our inference study for two reasons: 1) it has available emission data which does not possess the extreme stellar contamination issues seen for T-1 planets in transmission; and 2) compared to T-1b, which also has emission data (Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023), T-1c shows greater absorption in the $15\mu\text{m}$ bandpass relative to its expected dayside blackbody (Greene et al., 2023; Zieba et al., 2023), indicating that it is more likely to host an atmosphere than the hotter T-1b.

To identify the atmospheric sources and sinks that best reproduce the JWST emission observations of T-1c (Gillon et al., 2026; Zieba et al., 2023), we apply Bayesian ellipsoidal nested sampling using *PyMultiNest* (Buchner et al., 2014) as our sampler for the multi-modal nested sampling algorithm, *MultiNest* (Feroz et al., 2009, 2019). The forward model takes atmospheric boundary conditions, selected by *PyMultiNest*, as input and generates atmospheric profiles and spectra to compare with JWST data. We allow *PyMultiNest* to fit 7 dimensions: H_2O outgassing rate, CO_2 outgassing rate, atomic O top-of-atmosphere (TOA) escape rate, O_2 TOA escape rate, CO_2 TOA escape rate, CO dry surface deposition velocity, and trace SO_2 injection.

When conducting statistical inference, we begin with the fully self-consistent pipeline previously described (§2.2) — which automates the generation of a single atmospheric model

to convergence — but, because of the the need for thousands of forward model calls, we must improve the efficiency of our forward model by implementing an approximate climate scheme in place of the full *VPL Climate* model. Here we provide a description of the modifications to our self-consistent forward model pipeline that are used when applying the forward model in a Bayesian inference framework.

Similarly to our full pipeline, a given set of boundary conditions sampled by *MultiNest* is passed first to the *Atmos* photochemical model (Arney et al., 2016; Kasting et al., 1979; Meadows et al., 2018a). Following a converged run of *Atmos*, the offline surface pressure routine is called to determine if the atmospheric pressure has changed significantly, update the species profiles, and rerun *Atmos*; when conducting statistical inference, this rerun occurs if the pressure is found to change by $>5\%$, which is slightly relaxed in comparison to fully self-consistent pipeline which uses 3.5% .

For each forward model evaluation, the initial atmospheric state and climate profile are selected from the library of stable T-1c atmospheres found from completed grid sweeps using the fully self-consistent forward model pipeline (presented in Chapter 4). Although we ultimately want to select a climate profile based on the atmospheric composition and surface pressure, prior to a converged photochemical model the specific starting atmosphere is selected by identifying the stable model whose boundary conditions most closely match those specified for the current run. This match is quantified using a Euclidean distance metric:

$$d_e = \sqrt{\sum_i (\log(A_i) - \log(B_i))^2}, \quad (2.20)$$

where the distance is calculated by comparing i components of two vectors A and B . In the case of initial climate profile selection, we minimize the distance between the selected boundary conditions for the current run (A becomes Φ) and those of the precomputed stable run (B becomes ϕ). The previous stable run that minimizes the Euclidean distance (d_e) is selected for the current run’s starting point.

The selected initial atmospheric state is passed first to *Atmos*, along with the sampled boundary conditions, which is run to local convergence, defined as when stability is achieved for a timestep length exceeding 10^{17} s (i.e. >3 Gyr). The atmosphere is then passed to the surface pressure adjustment, which iterates back and forth with *Atmos* until both the photochemical model is converged and the surface pressure is changing by $\leq 5\%$. At this point, in the original self-consistent framework, the atmosphere would then be passed to *VPL Climate* to refine the temperature profile. However, as previously stated, the full climate model requires too much computation time to be employed in the statistical sampling method. Instead, we assess if the initially selected climate profile is still the best fit from the precomputed stable atmosphere library.

We will show that, when completing grid sweeps with the fully self-consistent forward model, all stable atmospheres of a particular compositional family posses similar pressure-temperature (P-T) profiles, which can be further narrowed down by the range of surface pressures (shown in Chapter 4). Thus, after a photochemical solution is found, we allow the climate profile to be updated based on the bulk composition and surface pressure. Whereas the initial climate state was found by minimizing the Euclidean distance metric between the atmospheric boundary conditions of the current run and a precomputed stable run,

after an atmosphere is converged through the photochemical model, we can use the actual composition and surface pressure to verify that the most optimal climate profile is selected. Thus, we then minimize the Euclidean distance between the species mixing ratios and surface pressure of the current run and the stable precomputed atmospheres, which is a better indicator of the P-T profile (Gialluca et al., 2026, In Review). Equation 2.20 is once again used, but A and B now represent the set of surface mixing ratios for each species and the total atmospheric surface pressure. If the closest matching P-T profile from the precomputed library is no longer the same as the one initially selected, the new best-fit profile is adopted and the model is rerun through the photochemical and surface pressure adjustment routines. Iteration between the photochemical portion of the pipeline and the selection of a P-T profile is continued until global convergence is achieved, when the best-fit P-T profile remains unchanged. If a model conducts more than 5 iterations without finding a consistent best-fit P-T profile, the run is rejected outright for instability.

Once the current atmospheric model is globally converged, we generate planetary spectra using *SMART* (Crisp, 1997; Meadows & Crisp, 1996; Robinson, 2017) and *LBLABC* (e.g., Meadows et al., 2018a) to compare with JWST data. As we are comparing our simulations to available T-1c emission data, which is currently confined to the $15\mu\text{m}$ bandpass (Gillon et al., 2026; Zieba et al., 2023), we constrain *SMART* to run only within $10 - 18\mu\text{m}$, which conserves computational efficiency.

2.3.1 Nested Sampling Process and Convergence

The Bayesian inference tool *MultiNest* (Feroz et al., 2009, 2019) is employed via *PyMultiNest* (Buchner et al., 2014) to identify solutions, or ‘modes’, within the input prior space through ellipsoidal nested sampling. In other words, the inference forward model framework is used by *MultiNest* in its likelihood function to generate atmospheric spectra using different samples of outgassing and loss processes. The spectra are then compared to the available emission and/or transmission data to determine the log-likelihood of a modeled atmosphere given the data using:

$$\ln\mathcal{L} = -\frac{1}{2} \sum_i \left(\frac{D_i - M_i}{\sigma_i} \right)^2, \quad (2.21)$$

where D_i is the data point from JWST for observation i , M_i is the atmosphere model point corresponding to the JWST observation, and σ_i is the uncertainty associated with the JWST observation. When conducting inference in Chapter 5, we compare models only to the available T-1c JWST emission data (Gillon et al., 2026; Zieba et al., 2023) because the large uncertainties and possible stellar contamination in transmission data (Radica et al., 2025).

As *MultiNest* runs, it calculates the remaining Bayesian evidence that could still reside in the unexplored parameter space, and compares that to what has already been collected to determine a stopping criterion. In Bayesian inference, the evidence (Z) is the probability of the data (D) given the model (M):

$$Z = P(D|M) = \int L(\Theta)\pi(\Theta)d^p\Theta, \quad (2.22)$$

where the evidence is found directly by integrating the likelihood ($L(\Theta)$) of a set of parameters (Θ) times their prior ($\pi(\Theta)$) over all dimensions of the parameter set (D_p dimensions). Nested sampling is an efficient means to evaluate the evidence of a model (by reducing the multidimensional integral, Eq. 2.22, to 1D) and conduct posterior inference, which we target in this study. *MultiNest* effectively explores the prior space while tracking 1) the evidence provided by its current set (Z_{curr}) of highest-likelihood samples (‘live-points’) and 2) the largest evidence contribution that could be made by the remaining, unexplored prior volume (Z_{remain}). The stopping criterion is when the remaining evidence could not change the current evidence by greater than a user defined tolerance (tol):

$$Z_{remain}/Z_{curr} < tol . \quad (2.23)$$

As we are using *MultiNest* to conduct posterior inference as opposed to comparison of multiple forward models, a higher tol is less influential for our case. We refer the reader to [Feroz et al. \(2009\)](#); [Feroz & Hobson \(2008\)](#) for an in-depth mathematical description of Bayesian nested sampling and the *MultiNest* algorithm specifically. Given the computational expense associated with our forward model, we present results that have achieved a tol of 10, though we conduct cross-validation to identify any potential undersampling. Cross-validation methods (using a K -fold approach) and techniques for extracting a solution set from the final posterior are described in the next section (§2.3.2).

2.3.2 Cross-Validation & Solution Mode Identification

With a completed *MultiNest* run yielding phase space samples and corresponding posterior probability, we perform a Gaussian Process (GP) Regression cross-validation, and then use two independent methods of extracting a final solution set. During a cross-validation, multiple kernels are trained and tested on posterior values to assess how well the posterior is constrained over the parameter space. We employ a K -fold validation technique, partitioning the *MultiNest* posterior dataset into K subsets (i.e., folds) and iteratively training each kernel on $K-1$ sets while evaluating on the final set, until each subset has served as the test set exactly once. In this work we use $K = 5$ folds and test five different kernels: a Radial Basis Function (RBF), Matérn 1.5 (once differentiable), Matérn 2.5 (twice differentiable), Rational Quadratic, and a Rational Quadratic plus Matérn 1.5 sum kernel. These kernels were selected to span a range of smoothness assumptions, from the infinitely differentiable RBF to the rougher Matérn 1.5, with the Rational Quadratic and sum kernel included to capture potential multi-scale structure in the posterior. For each kernel tested, we present the root mean squared error (RMSE) and R^2 value averaged across the results of each fold.

To prepare the full dataset for the cross-validation, we must apply a standardization to account for the considerable differences in scale across the seven dimensions explored by *MultiNest*. Since some parameters, like H_2O outgassing, may be many orders of magnitude larger than others, like effusion velocities, failing to account for this scale difference can bias the GP toward higher-magnitude dimensions. To account for this, we first transform parameters into log space, and then apply a standard scaler to normalize the data to zero mean and unit variance. This transformation also aides interpretability, as an RMSE of 1 would indicate that predictions are exactly 1 standard deviation away from the true posterior values in the normalized parameter space.

Following cross-validation, we used two methods to extract a final solution set: selection of the highest log-likelihood *MultiNest* samples and cluster identification via a Gaussian Mixture Model (GMM). The first method simply selects the top 10% of posterior samples ranked by log-likelihood, drawn from the *MultiNest* equal-weights posterior chain; we refer to the results of this first method as the “highest-likelihood solution set”. The second method employs a GMM to partition posterior samples into clusters using an expectation-maximization (EM) algorithm, identifying distinct solution families directly from the structure of the posterior distribution. When using a GMM, the number of clusters (i.e., ‘components’ or ‘solutions’) to assume must be specified a priori. To identify the optimal number, we test GMM fitting with 1 through 15 components and select the number that minimizes the Bayesian Information Criterion (BIC). The BIC is defined as:

$$BIC = -2 \log(L) + C \log(N) , \quad (2.24)$$

where L is the likelihood of the model, C is the tested number of components, and N is the number of samples. The first term of Eq. 2.24 rewards goodness-of-fit and the second term imposes a penalty for increasing number of components, balancing model fit and complexity.

Since the EM algorithm of a GMM is sensitive to initialization, the samples’ cluster assignments can vary across random states. To account for this, we test the GMM fitting process with 380 different random states and first identify the number of components that is most frequently selected as optimal by the BIC. For all GMMs that converge to this optimal component number, we then assess the consistency of their cluster partitioning by computing pairwise Euclidean distances (i.e., Eq. 2.20) between cluster means and standard deviations across all seven parameters. Finally, we select the GMM whose cluster solution set is closest to the centroid of this distance distribution; that is, the GMM that is most representative of the consensus partitioning across all random states is presented as the final cluster solution set. Note that the same log-transformed, zero mean and unit variance normalized posterior dataset used for the cross-validation analysis is used here, such that a Euclidean distance of 1 between two GMM solutions would indicate that their reported cluster means are separated by 1 standard deviation in the normalized parameter space.

2.4 Atmospheric Inputs & Boundary Conditions

For our first grid sweep analysis using the fully self-consistent forward model pipeline, we aim to generously encompass the phase space of plausible boundary conditions by defining broad ranges of source and sink flux rates informed by the literature. Transitioning to our statistical inference analysis, we allow the priors on boundary conditions to be informed by the result of our grid sweeps (presented in Chapter 4, and [Gialluca et al., 2026, In Review](#)). We discuss the specific input priors for our T-1c statistical inference analyses in the next sub-section (§2.4.1).

Across this dissertation, we focus on secondary atmospheres generated by water and CO₂ outgassing, with and without trace SO₂, based on the current best-fitting atmospheric cases from JWST observations ([Greene et al., 2023](#); [Ih et al., 2023](#); [Lim et al., 2023](#); [Lincowski et al., 2023](#); [Piaulet-Ghorayeb et al., 2025](#); [Radica et al., 2025](#); [Zieba et al., 2023](#)). The primary source for our atmospheres is either water outgassing alone, or mixed H₂O-CO₂

outgassing. All outgassing rates are constrained by [Thomas et al. \(2025\)](#), who used a magmatic outgassing model informed by solar system terrestrial bodies to define the region of outgassing rates that may be plausible for the TRAPPIST-1 planets. We allow outgassing rates to be sampled between the 2σ lower and upper values of the probability distribution given by [Thomas et al. \(2025\)](#) for a given planet.

There are 4 different sinks used in all atmosphere models: ozone (O_3) and hydrogen peroxide (H_2O_2) dry deposition at the surface, and atomic (O) and molecular oxygen (O_2) escape at the top of the atmosphere (TOA). Atmospheres that possess CO_2 outgassing also include CO_2 TOA escape and CO dry deposition. These loss processes were selected as common and strong sinks found on Earth and Mars (e.g., [Clifton et al., 2020](#); [Constant et al., 2008](#); [Gronoff et al., 2020](#); [Seinfeld & Pandis, 2016](#); [Stein et al., 2014](#); [Zahnle et al., 2008](#)) relative to other loss process related to water and its daughter photochemical products. Additionally, diffusion-limited H and H_2 escape are automatically included in *Atmos*, as is the case with past work using this photochemical model (e.g., [Lincowski et al., 2018, 2023](#); [Meadows et al., 2023, 2018a](#)). When defining deposition or effusion velocities, the following equation relates this velocity to total flux ($\text{cm}^{-2} \text{s}^{-1}$) for a species (s):

$$F_s = v n_s , \quad (2.25)$$

where v is replaced by the deposition (v_{dep}) or effusion (v_{eff}) velocity (cm/s), and n_s is the number density (cm^{-3}) of that species at the bottom or top layer of the atmosphere for surface deposition or TOA escape, respectively. For any given simulation, the deposition and effusion velocities of applicable sink processes are fixed, and the exact resulting loss flux will vary with the species' number densities (i.e., as composition and/or surface pressure change).

On Earth, deposition velocities of O_3 and H_2O_2 vary based on surface type (e.g., ocean, desert, forest, etc) and time of day. While continental O_3 deposition averages around 0.4 cm/s ([Seinfeld & Pandis, 2016](#)), this may be an overestimate for surfaces low in organic matter, such as the irradiated soils of the TRAPPIST-1 planets. For instance, the Sahara Desert shows values closer to 0.1 cm/s ([Clifton et al., 2020](#); [Güsten et al., 1996](#)). Snow-covered regions also exhibit lower O_3 deposition, with velocities typically between $0 - 0.1 \text{ cm/s}$ range ([Clifton et al., 2020](#); [Seinfeld & Pandis, 2016](#)). Over the Northeastern US, ozone deposition velocities were found to range from $0.7 - 0.8 \text{ cm/s}$ at midday to $0.1 - 0.2 \text{ cm/s}$ at night, while H_2O_2 deposition velocities ranged from $1.6 - 2 \text{ cm/s}$ at midday to $0.6 - 0.9 \text{ cm/s}$ at night ([Walcek, 1987](#)). Average H_2O_2 deposition velocities are about 0.5 cm/s over continents, 1 cm/s over oceans, and 0.32 cm/s over snow ([Seinfeld & Pandis, 2016](#)). [Zahnle et al. \(2008\)](#) models the past and present atmospheres of Mars using a 1D photochemical model, they found that the best fitting depositional velocities for ozone and H_2O_2 tend to be much lower than Earth, ranging from 0.01 to 0.03 cm/s for both gases. To account for this broad range of possibilities, our initial grid sweep simulation suites begin by testing deposition rates of 0.4 and 0.02 cm/s for both O_3 and H_2O_2 .

Carbon monoxide (CO) dry deposition on Earth is responsible for around $10 - 15\%$ of the global atmospheric CO loss ([Stein et al., 2014](#)). Depending on the surface composition, deposition velocities of CO range from negligible up to $\sim 0.1 \text{ cm/s}$ for modern Earth ([Constant et al., 2008](#); [Stein et al., 2014](#)). However, as CO deposition is strongly biologically mediated

on Earth, we assume that CO deposition will be less efficient in the abiotic environments considered in this study. Therefore, we restrict CO depositional velocities tested in this study to be <0.01 cm/s (Krissansen-Totton, *priv. comm.*).

The TOA escape boundary conditions of atomic O, O₂, and CO₂ (when applicable) are set by effusion velocities to allow the exact escape flux to respond to changing pressure and species concentrations during a simulation. This is necessary because specifying a fixed escape flux will prevent a simulation’s sink processes from responding to a changing atmosphere, which often leads to numerical instability. However, setting an effusion velocity can lead to widely ranging final escape fluxes due to the dependence on exact atmospheric composition, pressure, and mixing ratio profiles, which affects species’ number densities and ultimately the escape flux via Equation 2.25. In our results, we present the net escape fluxes of atmospheres found using this effusion velocity approach, and in discussion we assess if this inferred flux is reasonable in comparison to past studies.

A given effusion velocity may lead to widely varying escape fluxes, depending on final atmospheric composition. To provide some physical grounding for our ranges of effusion velocities, we consider some comparisons to Venus and Mars here. If we take the number density of atomic oxygen to be $\sim 10^{10} - 10^{11}$ cm⁻³ at 120 km ($\sim 10^{-7}$ bars) in Venus’ atmosphere (Brecht et al., 2012; Limaye et al., 2017), the effusion velocity would have to be $10^{-4} - 10^{-5}$ cm/s to achieve an escape velocity of $\sim 10^{24} - 10^{25}$ s⁻¹, similar to what is seen for neutral atomic oxygen sputtering and photochemical escape on Venus and Mars (Gronoff et al., 2020). In another example, if the number density of atomic oxygen at the exobase of Mars is taken to be $\sim 10^6 - 10^8$ (Qin, 2020), the effusion velocity would have to be 0.001 – 1 cm/s to achieve escape rates of $\sim 10^{24} - 10^{25}$ s⁻¹.

Given there is very limited data on the TRAPPIST-1 system, and that the heightened stellar activity may favor stronger escape processes (e.g., Howard et al., 2023), we begin by selecting effusion velocities near 0.01 – 1 cm/s and ultimately test effusion velocities as low as 10^{-8} cm/s. More specifically, for interior planets (T-1b, c, and d), we begin the initial simulation suite by testing effusion velocities of 0.01 and 1 cm/s for atomic oxygen, and 0.01 and 0.1 cm/s. For planets inside of and exterior to the habitable zone (T-1e, f, g, and h), we adopt 0.01 and 0.1 cm/s for atomic oxygen, and 0.01 and 0.05 cm/s for molecular oxygen effusion velocity in the initial simulation suites. When transitioning to atmospheres that also contain CO₂ outgassing, we initially test 0, 0.01, and 0.1 cm/s for CO₂ effusion velocities. As described previously, based on the results of the initial simulation suite, we allow sources and sink rates to vary as we target specific atmospheric pressures and stable atmospheric configurations. For example, if an atmosphere fails to be generated against strong loss processes, the effusion velocity may be slightly lowered in the subsequent simulation suite. For T-1e in particular, we test a much broader range of effusion velocities — with a lower limit down to 10^{-8} cm/s — to test if this would make a significant difference, but we found that it did not provide significantly different outcomes than an effusion velocity of 10^{-6} cm/s.

Table 2.3 provides the range of surface and TOA sink strengths that are tested across all grid sweep simulation suites in this study. For all stable and converged atmospheric models found in our H₂O and H₂O-CO₂ outgassing suites, we go on to explore SO₂ as a trace gas. For every stable atmosphere we add a fixed mixing ratio of SO₂ at the surface of 100 ppm, 0.1%, and 1%. These are then run through our photochemical-climate modeling pipeline, including the surface pressure re-adjustment routine. While SO₂ in these cases is set as a

Planet	Range of Tested Atmospheric Sink Strengths					
	Effusion Velocity [cm/s]			Deposition Velocity [cm/s]		
	O	O ₂	CO ₂	O ₃	H ₂ O ₂	CO
Innermost Planets (T-1b & c)	0.001 – 1.0	0.001 – 0.1	0 – 0.1	0.02 – 0.4	0.02 – 0.4	0 – 0.01
T-1d	0.001 – 1.0	10 ⁻⁶ – 0.1	0 – 0.1	0.02 – 0.4	0.02 – 0.4	0 – 0.01
T-1e	10 ⁻⁸ – 0.1	10 ⁻⁸ – 0.05	0 – 0.1	0.02 – 0.4	0.02 – 0.4	0 – 0.01
Outermost Planets (T-1f, g, & h)	0.001 – 0.1	10 ⁻⁶ – 0.05	0 – 0.1	0.02 – 0.4	0.02 – 0.4	0 – 0.01

Table 2.3: The strengths of TOA (effusion velocities, cm/s) and surface (deposition velocities, cm/s) atmospheric sinks tested across all grid sweep modeling suites. The innermost planets (T-1b & c) and the outermost planets (T-1f, g, & h) used the same ranges, but the two planets straddling the habitable zone (T-1d & e) were allowed to vary more widely (see text for more details). The final escape fluxes calculated from this effusion velocity approach are presented in detail and discussed further in the paper; in general the resulting escape fluxes are found to be within a reasonable range when compared to solar system bodies and past work on the TRAPPIST-1 system (e.g., [Dong et al., 2018](#)).

trace fixed mixing ratio, this does not significantly restrict the surface pressure, which still varies considerably due to the outgassing of bulk constituents and subsequent photochemical processes.

2.4.1 Input Priors for Statistical Inference

Informed by the results of our grid sweeps (presented in Chapter 4 and [Gialluca et al., 2026, In Review](#)), we focus statistical inference of T-1c atmospheres on a 7 dimensional input space: water outgassing rate, carbon dioxide outgassing rate, trace SO₂ mixing ratio in the bottom atmospheric layer, atomic O TOA escape effusion velocity, O₂ TOA escape effusion velocity, CO₂ TOA escape effusion velocity, and CO dry deposition velocity. We fix O₃ and H₂O₂ dry deposition velocity at 0.02 cm/s for statistical inference model runs because it is shown in [Gialluca et al. \(2026, In Review\)](#) that varying these inputs from 0.02 – 0.4 cm/s does not significantly affect simulation outcomes, and it is computationally favorable to reduce the number of input dimensions.

MultiNest natively samples all inputs from a D-dimensional unit hypercube (all parameters sampled from 0 to 1), thus a prior function is necessary to transform sampled inputs into their appropriate range. Since we use the precomputed stable atmospheres from our grid sweeps as a library for climate profiles, we constrain all inputs to be within the range of validity for the precomputed atmospheres. For most of the inputs, the sample (in the range 0 to 1) is transformed with a prior function of the following form:

$$S_{i,k} = S_{u,k} \times (Max_i - Min_i) + Min_i, \quad (2.26)$$

where $S_{i,k}$ is the sample of input i for simulation k , $S_{u,k}$ is the original unit hypercube sample from *MultiNest* (in the range 0 to 1), Max_i is the maximum allowed value for input i , and Min_i is the minimum allowed value. Equation 2.26 transforms a uniform sample between 0 – 1 into a uniform sample between $Min_i - Max_i$. In the case of CO₂ outgassing rate and trace SO₂ surface mixing ratio, we transform from a uniform sample to a sample in log space, for which we use the following form:

$$\log(S_{i,k}) = S_{u,k} \times (\log_{10}(Max_i) - \log_{10}(Min_i)) + \log_{10}(Min_i) , \quad (2.27)$$

this will bias the samples in that they will more often prefer the lower end of the range from $Min_i - Max_i$. The reason for doing this is that simulations with high CO₂ outgassing and/or high fractions of trace SO₂ were generally found to be less numerically stable in our forward model than those with lower amounts (Gialluca et al., 2026, In Review). This may be an artifact of the model and numerical stability with a greater number of inputs, rather than indication that atmospheres with these species are less probable. Regardless, using a log sampling approach allows the sampler to prefer more stable regions of parameter space at the beginning of a *MultiNest* run. In initial testing we found that this provided greater overall stability. Additionally, given that the 15 μ m data for T-1c has been found to disfavor significant CO₂ (Gillon et al., 2026; Zieba et al., 2023), the log prior for CO₂ also reflects that lower outgassing rates may be more probable.

Table 2.4 gives the range of validity (Min_i and Max_i) for each of our 7 input dimensions. These values are set to be the range of inputs that generated stable atmospheres in Gialluca et al. (2026, In Review). Note, the minimum value for CO₂ outgassing and trace SO₂ surface mixing ratio are set to small, near-zero values, since $\log_{10}(0)$ is undefined. Although the library of precomputed stable atmospheres includes models completely devoid of these species (exact zero values), the small values adopted for Min_i here are effectively negligible in our modeling framework. Another point to note is that a few stable atmospheres were found in our grid sweeps with O₂ effusion velocities of 0.1 cm/s, but this comprised only 2.3% of all stable atmospheres, which generally preferred much lower O₂ effusion velocities (often in the 0.001 – 0.01 range). Because of this, we leave the maximum allowed value for O₂ effusion velocity as 0.04 cm/s, to provide a tighter prior region. Finally, the prior region adopted for H₂O outgassing is between the 50th and 97.5th (upper 2 σ) percentiles of the outgassing distribution of Thomas et al. (2025); the full distribution (down to the lower 2 σ value) is explored in our grid sweep study, but it will be shown that higher H₂O outgassing rates are generally required to generate atmospheres.

3 Fitting Models to Data

Across this work, we place a particular focus on the level to which modeled planetary atmospheres fit JWST data, when available. For T-1b, emission data at 15 and 12.8 μ m (Ducrot et al., 2025; Greene et al., 2023) is available, as well as transmission data from JWST/NIRISS across 2 visits (Lim et al., 2023). For T-1c, emission data at 15 μ m is currently available (Zieba et al., 2023), as well as transmission data from JWST/NIRISS across 2 visits (Radica et al., 2025). For both T-1b and c, thermal phase curves further provide a 15 μ m nightside emission point, as well as another dayside 15 μ m measurement (Gillon et al., 2026).

	H ₂ O Flux (kg/yr)	CO ₂ Flux (kg/yr)	SO ₂ Trace Surface Mixing Ratio	O V _{eff} (cm/s)	O ₂ V _{eff} (cm/s)	CO ₂ V _{eff} (cm/s)	CO V _{dep} (cm/s)
Min Value (<i>Min_i</i>)	5.26×10 ¹⁰	1	10 ^{−30}	0.001	0	0	0
Max Value (<i>Max_i</i>)	5.50×10 ¹²	9.22×10 ⁹	0.01	1	0.04	0.1	0.03

Table 2.4: Priors on all seven parameters used in our Bayesian inference model. Ranges are selected to encompass values that led to any stable solution in [Gialluca et al. \(2026, In Review\)](#) (Chapter 4). Note, outgassing fluxes (H₂O and CO₂) are also informed by the distributions found in [Thomas et al. \(2025\)](#), but may be truncated based on the stability of the range found in [Gialluca et al. \(2026, In Review\)](#) (Chapter 4).

For T-1d, transmission data from JWST/NIRSpec across 2 visits are currently available ([Piaulet-Ghorayeb et al., 2025](#)). Finally, for T-1e, transmission data from JWST/NIRSpec across 4 visits are currently available ([Espinoza et al., 2025](#); [Glidden et al., 2025](#)). Note, the more recent data of [Allen et al. \(2025\)](#) was published after the results were completed in this work, while we use available data to analyze models conducted here, since these more recent T-1e observations would not change atmospheric interpretation or detection confidences, we stick to using the [Espinoza et al. \(2025\)](#); [Glidden et al. \(2025\)](#) data in our analyses.

When comparing an atmospheric model to available data we quote a “ σ confidence”, which is by definition the number of standard deviations from the mean of a normal two-sided probability distribution that corresponds to the p -value found from a χ^2 goodness-of-fit test. First we calculate the χ^2 value:

$$\chi^2 = \sum_i \left(\frac{O_i - M_i}{\sigma_i} \right)^2, \quad (2.28)$$

where O_i is the i^{th} data-point and M_i is the corresponding model point, and σ_i is the uncertainty on O_i . With χ^2 we can then calculate the p -value, which is the probability of obtaining a χ^2 value greater than or equal to the calculated value assuming degrees of freedom equal to the number of observations ($\nu = N_i$):

$$p = \mathbb{P}(\chi_\nu^2 \geq \chi_{\nu,obs}^2). \quad (2.29)$$

Finally we can use this p -value to arrive at a σ confidence that the model matches the data. In practice, we calculate these values using the Scipy.stats.chi2 package cumulative distribution function ([Virtanen et al., 2021](#)).

3.0.1 Correlation Coefficient

Given that standard ‘goodness-of-fit’ data-model comparisons neglect the correlation of adjacent wavelength bins, we also employ the Pearson Correlation Coefficient (PCC) as an additional metric to compare modeled spectra to data in our grid sweep analyses. The PCC may provide sensitivity to multiple, correlated, spectral features from a given molecular species through the slope of the spectra. Traditionally when matching individual models to

observation outside of a full retrieval, the χ^2 , p -value, and/or σ fit methods described above are used. However, these methods treat each data-model point independently, when in reality spectral features are correlated; for example, if significant CO_2 is present in an atmosphere, one should see an absorption feature above the baseline at both 4.3 and $15\mu\text{m}$. Thus, more information on how the model fits the data can be discerned from considering the general trend of the spectrum as a whole. In other words, a good fitting model should be positively correlated to the data points (i.e., when the data points indicate a larger transmission depth, the model's transmission depth should also increase).

To quantify the additional information that can be derived from analyzing how a modeled spectra correlates to the observations, we use the PCC. The PCC ranges from -1 to 1 with -1 being perfectly negative correlated, 0 being no correlation, and 1 being perfectly positively correlated. Ideally, a good fitting model should have a PCC approaching 1, indicating the model predicts absorption when there is potential absorption seen in the data compared to its baseline. We use the PCC to compare modeled transmission spectra to JWST data in the grid sweep analyses of this dissertation (applicable for T-1b, c, d, and e). Since emission photometry only provides 1 data point, a correlation across a dataset cannot be established.

For a single model to data comparison, the PCC is defined as:

$$\rho_{CC} = \frac{N_i \left(\sum_i O_i M_i \right) - \left(\sum_i O_i \right) \left(\sum_i M_i \right)}{\sqrt{\left[N_i \left(\sum_i O_i^2 \right) - \left(\sum_i O_i \right)^2 \right] \left[N_i \left(\sum_i M_i^2 \right) - \left(\sum_i M_i \right)^2 \right]}}, \quad (2.30)$$

where O_i is the i^{th} observation, M_i is the corresponding model point, and N_i is the total number of observations. Note, Equation 2.30 does not inherently account for when there are observational uncertainties (σ_i). To fold in the observational uncertainty for a given model-to-data comparison, we first take 500 randomly sampled observational datasets, taken assuming each data point has an asymmetrical normal distribution defined by that point's value and upper and lower uncertainty. Then, for each of the randomly sampled datasets, we calculate the PCC with the particular modeled spectrum being tested (calculating 500 PCCs), and we finally report the 50th percentile value of the set of PCCs as the answer. Since this metric has not been commonly used in this field, we provide a proof of concept for how this can maximize information in Chapter 4's Appendix 7.1.

4 Calculating Available Gibbs Free Energy

Since the atmospheres we generate can produce high chemical disequilibria (e.g., through high CO), for the atmospheres presented in the grid sweep analyses of this dissertation, we explore the potential for biosignature false positives by quantifying the available Gibbs free energy (Krissansen-Totton et al., 2016). Here the available Gibbs free energy is defined as the Gibbs free energy of an atmosphere minus that of the atmosphere's constituents reacted to equilibrium, following the method of Krissansen-Totton et al. (2016):

$$\Phi = G_{(T,P)}(n_i) - G_{(T,P)}(\bar{n}_i) . \quad (2.31)$$

The Gibbs free energy of the atmospheric constituents reacted to equilibrium is found by minimizing the Gibbs free energy equation, assuming a constant temperature and pressure (Eq. 1 from Krissansen-Totton et al., 2016):

$$G_{(T,P)} = \sum_i^N \left(\frac{\partial G}{\partial n_i} \right)_{(T,P)} n_i , \quad (2.32)$$

where n_i is the number of moles of each gas, i , and N is the total number of chemical species present. We refer the reader to Krissansen-Totton et al. (2016) for a detailed description of how the Gibbs free energy is derived and calculated. While Krissansen-Totton et al. (2016) considered multiphase calculations of an atmosphere-ocean system for Earth, we only consider a gaseous phase for the atmospheres here. Moreover, while Krissansen-Totton et al. (2016) provided a public MATLAB model for this calculation, we have created an equivalent model entirely in Python, which we also make publicly available on GitHub¹; when using this Python model, the original text of Krissansen-Totton et al. (2016) as well as this dissertation should be cited. The Python implementation of the Krissansen-Totton et al. (2016) model is validated for the Mars and Jupiter case against the original MATLAB source code.

¹<https://github.com/mgialluca/ChemDisequilibriumPython>

CHAPTER 3

THE IMPLICATIONS OF THERMAL HYDRODYNAMIC ATMOSPHERIC ESCAPE ON THE TRAPPIST-1 PLANETS

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1 Summary

JWST observations of the 7-planet TRAPPIST-1 system will provide an excellent opportunity to test outcomes of stellar-driven evolution of terrestrial planetary atmospheres, including atmospheric escape, ocean loss and abiotic oxygen production. While most previous studies use a single luminosity evolution for the host star, we incorporate observational uncertainties in stellar mass, luminosity evolution, system age, and planetary parameters to statistically explore the plausible range of planetary atmospheric escape outcomes. We present probabilistic distributions of total water loss and oxygen production as a function of initial water content, for planets with initially pure water atmospheres and no interior-atmosphere exchange. We find that the interior planets are desiccated for initial water contents below 50 Earth oceans. For TRAPPIST-1e, f, g, and h, we report maximum water loss ranges of $8.0^{+1.3}_{-0.9}$, $4.8^{+0.6}_{-0.4}$, $3.4^{+0.3}_{-0.3}$, and $0.8^{+0.2}_{-0.1}$ Earth oceans, respectively, with corresponding maximum oxygen retention of 1290^{+75}_{-75} , 800^{+40}_{-40} , 560^{+30}_{-25} , and 90^{+10}_{-10} bars. We explore statistical constraints on initial water content imposed by current water content, which could inform evolutionary history and planet formation. If TRAPPIST-1b is airless while TRAPPIST-1c possesses a tenuous oxygen atmosphere, as initial JWST observations suggest, then our models predict an initial surface water content of $8.2^{+1.5}_{-1.0}$ Earth oceans for these worlds, leading to the outer planets retaining >1.5 Earth oceans after entering the habitable zone. Even if TRAPPIST-1c is airless, surface water on the outer planets would not be precluded.

2 Brief Introduction

In this chapter, we explore the volatile evolution and loss history of all seven TRAPPIST-1 planets by modeling water loss through hydrodynamic thermal atmospheric escape from the system’s formation to habitable zone entrance or present-day. We leverage the computationally efficient planetary evolution model, VPlanet (Barnes et al., 2020), with developed support scripts (Vconverge) to automatically run simulation suites to convergence, here we explore the full observational uncertainty of the stellar evolution (Birky et al., 2021) and planetary parameters (Agol et al., 2021) of the TRAPPIST-1 system. To define the plausible phase space of water loss and oxygen production outcomes, we conduct hundreds of thousands of simulations of the water evolution history of the TRAPPIST-1 planets across a grid of initial water contents from 1 terrestrial ocean (TO) to 500 TO - spanning the full range that has been suggested as plausible in the literature (Acuña et al., 2021; Agol et al., 2021; Raymond et al., 2022; Schoonenberg et al., 2019). A terrestrial ocean, or Earth ocean, is our standard unit of measurement for water content and is equivalent to 1.39×10^{21} kg. Though Krissansen-Totton & Fortney (2022) adopted a similar statistical approach considering the system constraints from Birky et al. (2021) and Agol et al. (2021), our study conducts a greater number of simulations to more comprehensively explore the phase space of initial

water content, although at the expense of a coupled atmosphere and interior. We present predictions with 1σ uncertainty on water loss as a function of initial water abundance for each TRAPPIST-1 planet. This study additionally identifies the maximum water loss possible for the HZ planets regardless of increasing initial water mass, assuming initially pure water atmospheres and no exchange with the interior. Furthermore, given this maximum water loss and our understanding of oxygen drag during escape, we calculate the maximum amount of abiotic oxygen that could be produced through this process, with perfectly ineffective oxygen sinks at the surface, to provide upper limits on total atmospheric oxygen build-up.

Through this statistical study of all 7 known planets in the system, escape evolution as a function of orbital distance is explored, methods of inferring system evolution from observation are developed and demonstrated, model intercomparisons are explicitly quantified (Krissansen-Totton & Fortney, 2022), and we begin to interpret the most recent JWST observations (Greene et al., 2023; Zieba et al., 2023) in the context of our findings. To infer system evolution, we show how our knowledge of water loss over time can be used in conjunction with present-day water mass fraction (WMF) measurements of the TRAPPIST-1 planets to retrieve plausible evolutionary histories and probable initial water contents. The retrieval of evolutionary history will aid in developing a relationship between initial and final water content that can connect formation models to observations. In regards to JWST, we consider recent observations (Greene et al., 2023; Zieba et al., 2023) in the context of our results by analyzing the planets individually, and then by showing the significant additional information that can be discerned when considering multiple bodies in the system and using a comparative planetology approach. In particular, we provide insights into initial water content of the system and current plausible conditions on planets that have yet to be observed.

Section 3 presents the key results of our study, including the evolutionary pathways observed in our simulations (§3.1), the full statistical spread of all models (§3.2), identification of the most probable initial water content to reproduce final water mass fractions presented in Agol et al. (2021) (§3.3.1), quantification of oxygen retention efficiency (§3.4), and a comparison of our results to a similar study published in Krissansen-Totton & Fortney (2022) (§3.5). The interpretation, significance, and limitations of these results and comparison to past work is discussed in Section 4, notably including an analysis of recent JWST observations in the context of our study (§4.3.2). We summarize our conclusions in Section 5. Please note, in referring to individual planets, we adopt the shorthand of ‘T1- i ’ for ‘TRAPPIST-1 i ’, where i would refer to the planet in question (b, c, d, e, f, g, or h).

3 Results

We first describe the possible pathways of escape observed in our simulations for each planet through time, and how they change for different initial water contents (§3.1). We then present probabilistic distributions of final water loss and oxygen production for each planet as a function of initial water content (§3.2). Finally, we show the results of analyses performed with the data, including methodology for predicting initial water content from a known final water content (§3.3.1), efficiency of oxygen production through escape (§3.4), and a

comparison to existing work with more comprehensive interior modeling (Krissansen-Totton & Fortney, 2022) to contextualize the atmospheric escape calculations of both studies (§3.5).

3.1 Escape Through Time

Here, we describe the 6 distinct evolutionary pathways that the TRAPPIST-1 planets displayed in our model, due to combinations of escape physics, assumed initial water, and the interactions between the host star evolution and planetary properties (Figure 3.1). A given simulation’s behavior as the host star luminosity and XUV evolves is primarily contingent on initial water content and orbital distance, but noticeable effects can also be attributed to the planet’s mass and radius. Understanding the possible mechanisms of escape a planet could experience as a function of stellar evolution and planetary properties helps predict likely observables. Note, that "Oxygen Retained" (used on the y-axis label of Figures 3.1, 3.2 and 3.3) refers to the oxygen that was produced and retained through the photolysis and thermal escape of water, when considering loss through hydrodynamic drag as the only oxygen sink.

There are 3 possible states a planet may be in when the hydrodynamic escape phase ends, here termed “end states”: hydrodynamic thermal escape is halted by complete desiccation (Figure 3.1, left column), escape is halted by sufficient decrease in incident XUV marked by entrance to the habitable zone (HZ) (Figure 3.1, middle column), or escape never ends and is active at present day (Figure 3.1, right column). Within these cases, we can also consider whether the planet experienced diffusion-limited escape, or if it remained in the energy-limited regime for the duration of the simulation. As diffusion is responsible for mass fractionation, which may be observable (Lincowski et al., 2019), knowledge of whether or not a planet may have experienced diffusion-limited escape is important for predicting the likelihood of fractionation signals in the planetary spectrum.

Planetary desiccation is due to an interplay between the planet’s initial water content and its accumulated stellar insolation. Desiccation may therefore be experienced by any planet in the system regardless of orbital distance, as those planets with lower initial water inventories are more likely to become desiccated, in addition to those with larger stellar insolation. If a planet becomes desiccated, it will pass the point where the mixing ratio of water is less than that of free oxygen (i.e., the “diffusion switch”); thus, by definition planets that become desiccated will last be in the diffusion-limited escape regime.

As an M dwarf’s luminosity fades with time, a planet once interior to the habitable zone may enter it (Luger & Barnes, 2015), and it is assumed that this will shut off hydrodynamic escape due to the formation of a cold trap that prevents sufficient water from reaching the exobase (Kasting, 1988). Only the outer planets (beyond TRAPPIST-1 d) will enter the HZ and experience this shut-off mechanism, thus it is primarily dependent on orbital position. We find the inner edge of the HZ reaches planets T1-e, f, g, and h at roughly ~ 380 Myr, ~ 170 Myr, ~ 100 Myr, and ~ 50 Myr, respectively, thus there is a short amount of time for the planets to lose water relative to the age of the system. Consequently, depending on their initial water inventories, these planets may or may not have experienced diffusion-limited escape, with lower initial water contents more likely to reach the diffusion switch before HZ entrance.

In the last end state, escape is never halted before the age of the system is reached, and

the planet retains water and active escape up to present-day. Since the planets beyond TRAPPIST-1 d will have entered or passed beyond the habitable zone by the present day, simulations that end with active escape can only occur for interior planets. This end state is primarily dependent on initial water and typically only occurs for large initial water contents of $>30 - 60$ TO, depending on orbital distance. Planets that follow this trajectory can experience diffusion-limited escape or stay in the energy-limited regime for the entire simulation, which is also dependent on initial water content and integrated insolation over time.

As uncertainty in the stellar evolution can affect what pathway a particular planet takes, and uncertainty in planetary mass and radius can sway borderline cases, this work leverages over 700,000 simulations to explore the full uncertainty space. The predicted final states of the planets and associated uncertainty from the culmination of all simulations is described in the following section.

3.2 Statistical Outcomes of Simulation Final States

Here we present the distributions from all simulations of water loss and oxygen production for each planet as a function of initial water content (Figures 3.2 and 3.3). Figure 3.2 shows the predicted final water loss (top row) and oxygen retained (bottom row) for the TRAPPIST-1 interior planets (T1-b, c, and d). For low initial water contents ($1 - 20$ TO, left column), the interior planets are completely desiccated, enabling large amounts of oxygen production; T1-c retains the most oxygen against atmospheric escape, followed by d and then b. At larger water contents, T1-c continues to retain the most oxygen, but T1-b begins to retain more than T1-d due to T1-b's greater cumulative water loss at large initial reservoirs. T1-b, c, and d begin to avoid desiccation and retain fractional amounts of an ocean at initial water contents of 60, 50, and 30 TO, respectively.

For higher initial water contents ($30 - 500$ TO, right column), the interior planets' water loss curves begin to flatten, approaching a maximum possible water loss value. Maximum possible water loss here refers to the maximum amount of water a planet can lose given its maximum possible simulation time (the system age for interior planets, the time to the habitable zone for exterior planets) and sufficiently large water contents, such that adding more initial water would negligibly affect the predicted water loss. As water loss directly correlates with oxygen production, we also see maximum values for oxygen production and retention after thermal escape corresponding to maximum possible water loss. T1-d clearly displays this flattening off behavior indicating a maximum possible water loss of ~ 90 TO and oxygen production of $\sim 15,000$ bars. The continuing upward trend of water loss and oxygen production for T1-b and c suggest that the maximum possible water loss is first achieved for initial contents larger than those considered in this work (>500 TO), but we can conclude the maximum possible water loss of T1-b and c is greater than ~ 250 TO and ~ 230 TO, respectively.

When considering only the balance of oxygen production and loss through thermal escape of water atmospheres, we may quantitatively explore the tendency of the planets to retain the oxygen they produce, or become completely airless. In some simulations with very low initial water, oxygen drag may be so efficient that only a negligible (<1 bar) atmosphere remains post-escape, even without the consideration of additional oxygen sinks (e.g., [Schaefer](#)

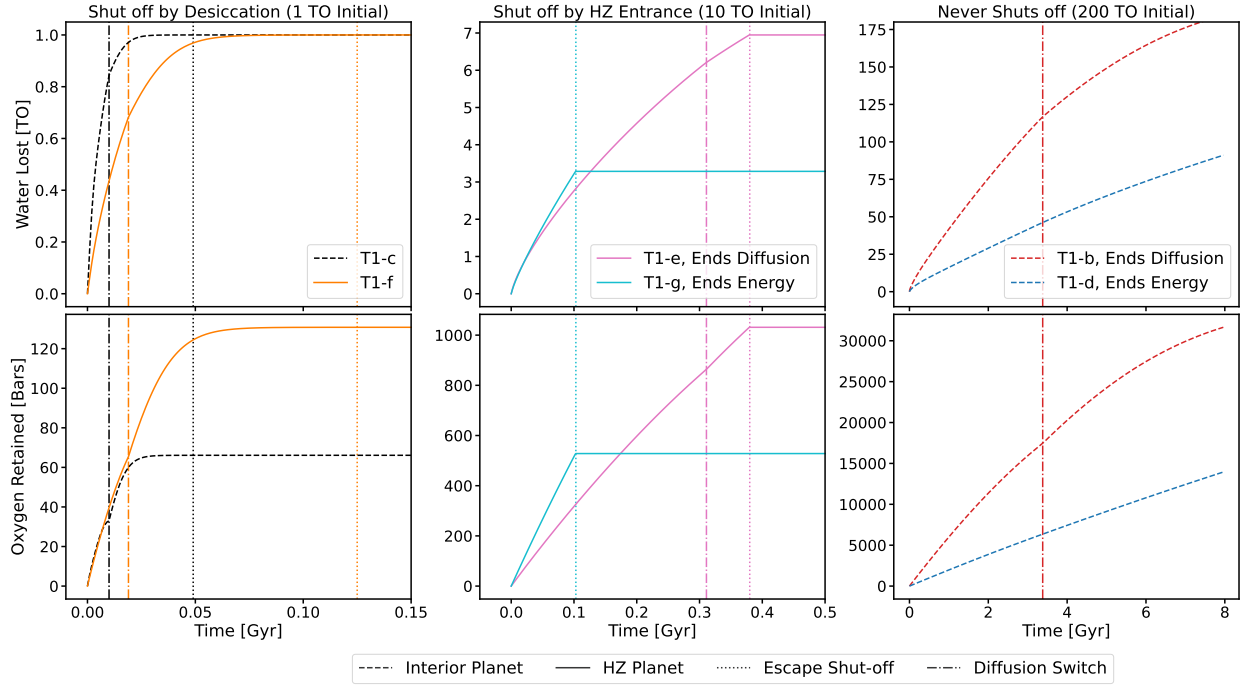


Figure 3.1: Illustration of the possible pathways the TRAPPIST-1 planets can take through escape physics in our model. Interior planets are denoted by dashed curves and habitable zone (HZ) planets are denoted with solid curves. Escape shut off times are shown by vertical dotted lines and times of switches from energy-limited to diffusion-limited escape are shown by vertical dot-dashed lines. **Left Column:** Escape is halted by complete planetary desiccation, for an interior planet, T1-c (black), and for a HZ planet, T1-f (orange), both with 1 TO initial water inventory. In these cases the atmospheric water is removed entirely, and the planet is last in diffusion-limited escape before the simulation halts. **Middle Column:** Simulations of HZ or outer planets where escape is halted by entrance to the HZ and the subsequent formation of a cold trap, all for initial water inventories of 10 TO. In this case escape could end in either the diffusion-limited (for T1-e, pink) or energy-limited (for T1-g, teal) regime. **Right Column:** Escape never shuts off as the planetary water reservoir is sufficiently large to sustain ongoing escape through the systems lifetime. This end state can only occur for interior planets (and results for T-1 b and d with an initial water inventory of 200 TO are shown here) as planets in or beyond the HZ have escape shut off by the formation of a cold trap. Once again, escape could end in either the diffusion-limited (for T1-b, red) or energy-limited (for T1-d, blue) regime, depending on total received insolation and initial water inventory. **Top Row:** Shows water lost (in TO) over time for each of the column cases previously described. **Bottom Row:** Shows oxygen produced (in bars) over time for each of the column cases previously described.

et al., 2016); for an initial content of 1 TO, $\sim 19\%$, $\sim 2.0\%$, and $\sim 2.5\%$ of T1-b, c, and d simulations, respectively, were completely airless. This number drops to less than 1% for all planets by an initial content of 5 TO.

Figure 3.3 shows the water loss and oxygen production results for the HZ and outer planets (T1-e, f, g, and h) with the same layout as Figure 3.2. The outer planets rarely or never experience desiccation above a threshold initial water inventory; T1-e is desiccated for initial water up to 2 TO, while T1-f is only desiccated for 1 TO initial. T1-g is nearly desiccated for 1 TO, only retaining on the order of 10^{-5} TO, but T1-h is never predicted to be desiccated for the initial water contents considered here (≥ 1 TO).

As HZ entrance halts escape on the outer planets, there is only a short time frame prior to entering the HZ (approximately 50-380 Myr) in which these planets can experience massive water loss through thermal hydrodynamic escape, which significantly limits their maximum possible water loss, and oxygen buildup and retention. T1-e, f, g, and h display maximum possible water losses of $8.0^{+1.3}_{-0.9}$, $4.8^{+0.6}_{-0.4}$, $3.4^{+0.3}_{-0.3}$, and $0.8^{+0.2}_{-0.1}$ TO, respectively, with corresponding maximum possible oxygen retention amounts of 1290^{+75}_{-75} , 800^{+40}_{-40} , 560^{+30}_{-25} , and 90^{+10}_{-10} bars, respectively. For initial water inventories above 4 TO, water loss amounts tend to decrease with increasing orbital distances, with T1-e losing the most, followed by f, g, and h. However, for low initial water contents (≤ 2 TO), the planets lose comparable amounts of water, but T1-g retains the most oxygen due to its lower incident radiation followed by f, e, and then h. At an initial water inventory of 3 TO, T1-g moves to retain less oxygen than T1-f and e, and by 4 TO the ordering of the planets' oxygen retention tends back towards their orbital distance ordering as the closer planets lose more water overall and thus build-up more oxygen.

Unlike the interior planets, the outer planets are rarely found to lose all produced oxygen. At an initial content of 1 TO, less than 1% of simulations for all outer planets retain < 1 bar of oxygen. For all 7 planets, the differences in oxygen retention ordering are influenced by the XUV environment and planetary gravity. In Section 4, we discuss these water loss (§4.1) and oxygen build-up (§4.2) results, along with the broader implications and importance.

3.3 Predicting Initial Water Content

A fundamental limitation to our understanding of planetary evolutionary processes is that the atmospheric histories of exoplanets are not directly observable; however, they may be inferred from other measurable quantities. Here, we show two different approaches to inferring initial water content: first by using predictions of the present-day water mass fraction of the planets (Agol et al., 2021) (§3.3.1), and then by using constraints on atmospheric oxygen content of the interior two planets inferred from the most recent JWST observations (Greene et al., 2023; Zieba et al., 2023) (§3.3.2).

3.3.1 Using Present-day Water Mass Fractions

Within our model and its limitations, we have shown a direct relationship between the initial and final water contents of the TRAPPIST-1 planets (Figures 3.2 & 3.3); thus, it is possible to take a known or predicted final water content and determine the initial water content our model predicts that is most likely to produce that final state. As our models only consider one

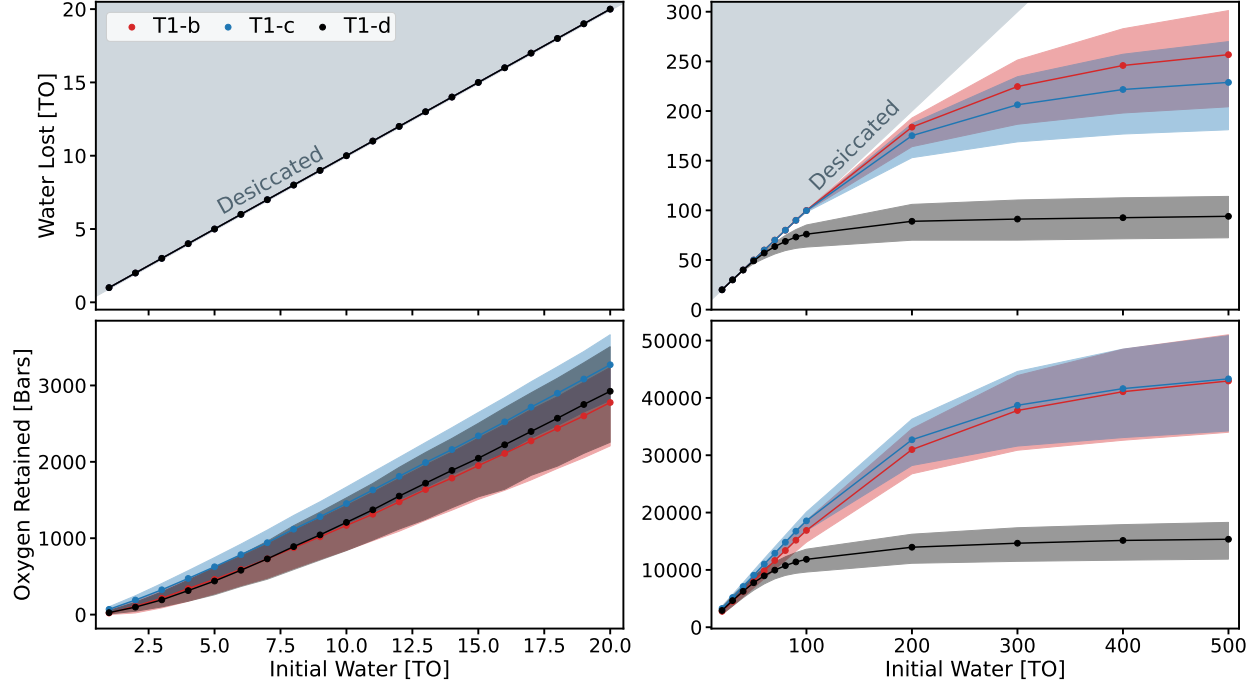


Figure 3.2: The predicted final water loss and final oxygen produced and retained as a function of initial water content for the TRAPPIST-1 interior planets T1-b (red), c (black), and d (blue). **Top Row:** Water lost (in TO) versus initial water (in TO); the shaded blue-grey region indicates where desiccation occurs. For water contents in the upper left panel, all three planets are desiccated and thus their curves are overlapping. **Bottom Row:** Oxygen produced and retained (in bars) versus initial water. **Left Column:** Low initial water contents (1 – 20 TO). **Right Column:** High initial water contents (30 – 500 TO). Shaded regions give the 1σ uncertainty ranges (set by the 16th and 84th percentile values of the final state distributions).

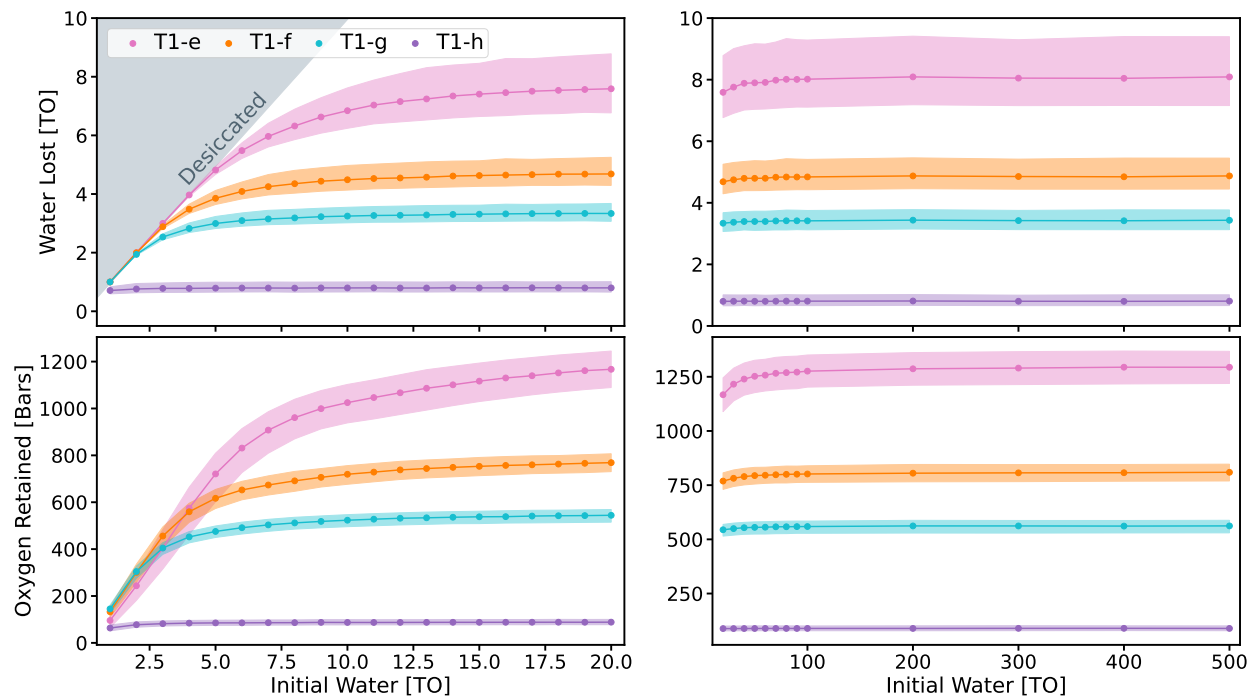


Figure 3.3: The predicted final water loss and final oxygen produced and retained as a function of initial water content for the TRAPPIST-1 habitable zone and outer planets T1-e (pink), f (orange), g (teal), and h (purple). The layout of the figure is the same as Figure 3.2.

evolutionary process (atmospheric escape driven by evolving stellar conditions), we caution that this analysis is meant to be a proof of concept. Our results are dependent on our model assumptions and limitations, as well as the assumptions made in the final state predictions we adopt.

In this analysis, we use the present-day water mass fraction predictions for each of the TRAPPIST-1 planets from [Agol et al. \(2021\)](#), which are derived from observationally constrained planetary densities, assuming an Earth-like core mass fraction of 32.5%. To calculate these water mass fractions, [Agol et al. \(2021\)](#) assumes all water on the planets is on the surface; steam ([Turbet et al., 2020b](#)) and condensed ([Dorn et al., 2017](#)) water mass-radius relationships were used for the interior (T1-b – d) and outer (T1-e – h) planets, respectively. As any surface water on the interior planets is expected to be vaporized ([Turbet et al., 2020b, 2019](#)), they conclude the interior planets should have water mass fractions drastically less than 0.01 wt%. Since a broad range of our initial water contents would result in this desiccated state for the inner planets, we cannot constrain their most probable initial water contents from this present day desiccated state alone; thus, we only attempt to constrain initial water abundance for the outer planets. The predicted present-day water constraints we adopt for the outer planets T1-e, f, g, and h are given in Table 3.1 (from Table 9 in [Agol et al., 2021](#)).

Body	Water Mass Fraction [H ₂ O wt%]
T1-e	$2.9^{+1.7}_{-1.5}$
T1-f	$4.5^{+1.8}_{-1.2}$
T1-g	$6.4^{+2.0}_{-1.6}$
T1-h	$5.5^{+4.5}_{-3.1}$

Table 3.1: Present-day water mass fraction constraints for the outer planets (T1-e, f, g, and h) that we use to predict most probable initial water content in our model. These constraints are taken from [Agol et al. \(2021\)](#) when assuming an Earth-like CMF of 32.5%, and are not definitively the true water mass fractions of the planets.

The method described in Appendix 7.1 is used to determine the initial water content most likely to produce these predicted final water contents in our model. Briefly, the present-day water predictions are first modeled with a gamma probability density function (PDF); we then sum the individual simulations’ values on that PDF and normalize for the number of simulations per initial water content to get a likelihood of that initial content given our predicted final state. Figure 3.4 shows the likelihood versus initial water content per planet. The peaks of these curves indicate the initial water content on our sampling grid that best recreated the predicted final states; for T1-e, f, g, and h these are 90, 200, 300, and 80 TO, respectively.

We further derive the 50th percentile value of probable initial water with uncertainty for T1-e, as a proof of concept. To find the most probable initial water content predicted by our model with associated confidence intervals, we need to interpolate across the curves in Figure

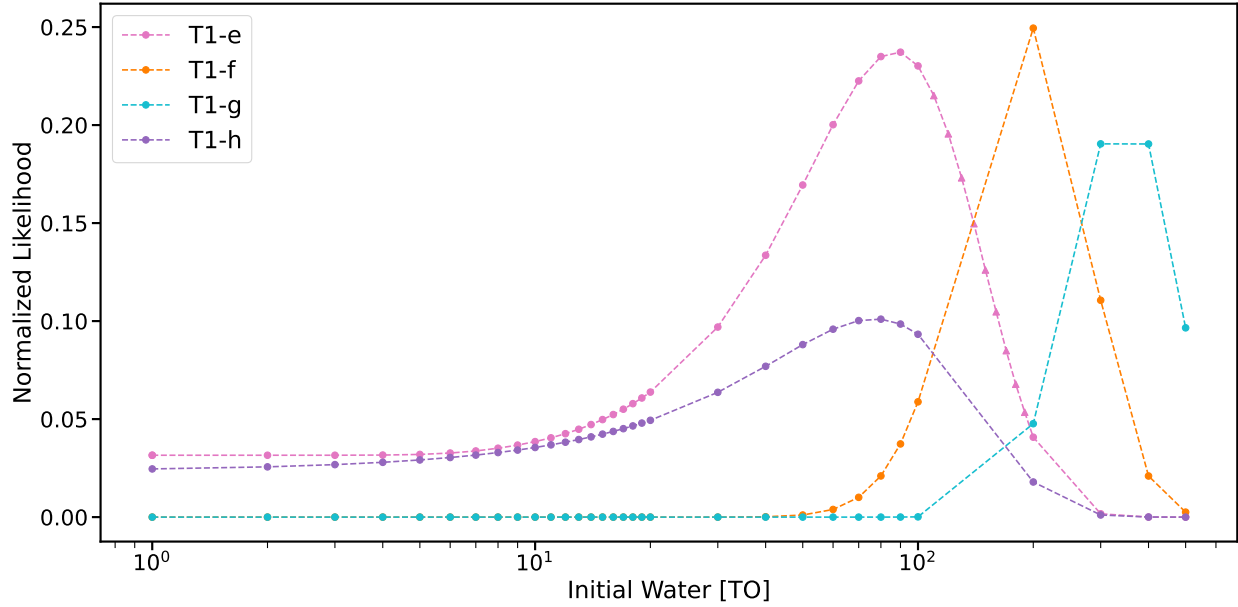


Figure 3.4: The likelihood of each initial water content (in TO) needed to reproduce the predicted present-day water contents from Agol et al. (2021) for each of the outer planets. The peaks denote the initial water content on our sampling grid most likely to produce the final content in our predictions. An additional 9 simulation suites were ran for T1-e only, between 100 – 200 TO to fill out a smooth, continuous curve, and results from these additional simulations are denoted by triangle markers.

3.4, which must possess enough data to be smooth and continuous. Many of the planets we’ve considered do not possess smooth and continuous curves, and adding more data to these requires many additional simulation suites and computational expense; because of this, and the inherent uncertainty in our predictions, we complete this additional analysis for T1-e only as proof of concept. To obtain a continuous curve for T1-e, an additional 9 simulation suites were completed for initial water contents between 100 – 200 TO (step size of 10 TO); additional data points for T1-e are shown by a triangle marker in Figures 3.4 & 3.5. These additional simulation suites are only considered in this initial water content analysis, as their inclusion in the results presented in Section 3.2 would not change the conclusions.

The interpolation for T1-e is accomplished with a modified Riemann sum, illustrated by Figure 3.5, to determine the 50th percentile value of predicted initial water content and associated 1 σ and 2 σ confidence intervals (see Appendix 7.1 for mathematical description). The 1 σ confidence interval of most probable initial water content to produce our present-day water content prediction for T1-e is $90.6^{+70.6}_{-37.2}$ TO, and the 2 σ confidence value is $90.6^{+155}_{-71.3}$ TO. Applications and importance of this method are further discussed in Section 4.3.1.

3.3.2 Using Constraints on Atmospheric Oxygen Abundance

Although the statistical inference technique (§3.3.1) can produce an upper limit on initial water abundance, a more refined estimate can be obtained by deriving tighter constraints from existing and future observations of atmospheric oxygen abundance on T1-b and c. Re-

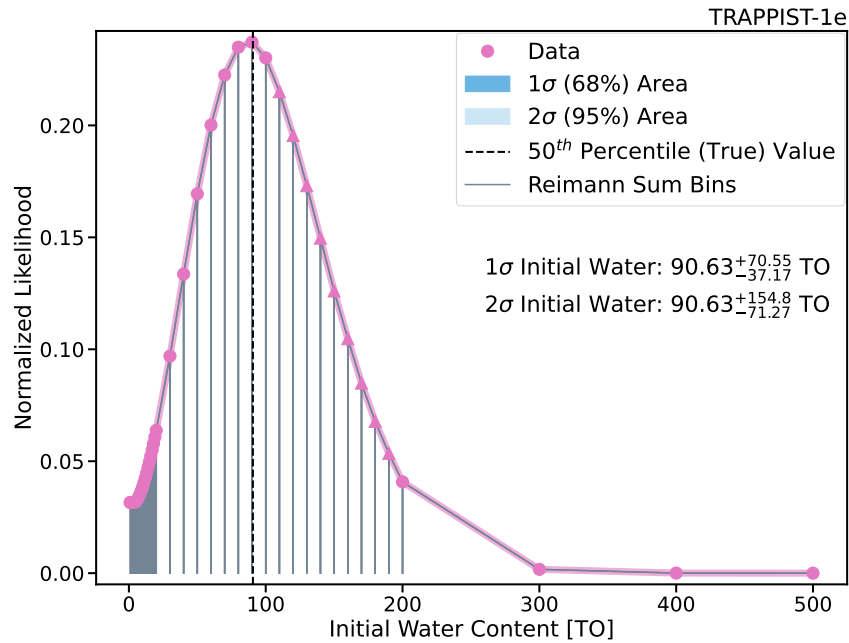


Figure 3.5: An illustration of the method used to determine the most probable initial water content for T1-e that would reproduce our predicted present-day content from [Agol et al. \(2021\)](#) (Table 3.1). Same layout as Figure 3.4 but with linear x-axis scaling; the y-axis is the likelihood that each initial water content (in TO; x-axis) produces the desired final state. The data points that were simulated are shown by the pink points, the bins used in the Riemann sum are shown in grey, the determined 50th percentile or true predicted value is shown by the vertical dashed black line, and the 1 σ and 2 σ confidence intervals are shown by the shaded dark and light blue regions, respectively. The low initial water contents (1 – 20 TO) are much more finely spaced (step size of 1 TO) which is why the Riemann sum bin widths are not resolvable there. Lines connecting data points are used for the tops of the Riemann sum bins.

cently, [Greene et al. \(2023\)](#) used JWST/MIRI to obtain a blackbody brightness temperature of $T_B = 503^{+26}_{-27}$ K for T1-b from secondary eclipse observations taken at $15\ \mu\text{m}$, which they find to be an excellent match to the 508K theoretical prediction of dayside temperature for an airless world with no heat redistribution. If a significant atmosphere was present, then the subsequent redistribution of heat from the dayside to nightside, and/or absorption from atmospheric CO_2 , would result in an average dayside temperature at $15\ \mu\text{m}$ that is significantly lower than that observed. [Greene et al. \(2023\)](#) therefore conclude that T1-b likely does not have a substantial atmosphere today. This observation is also consistent with nearly half of all evolutionary model runs from [Krissansen-Totton & Fortney \(2022\)](#), which predict complete atmospheric erosion on T1-b across their considered range of initial water ($0.7 - 300$ TO).

The observational constraint that T1-b is likely airless today can be used with our grid of atmospheric evolutionary outcomes to identify limits on the planet’s initial surface water. Considering only the apparent lack of water, our model predicts the planet must have begun with ≤ 60 TO to be in a desiccated present-day state. Although water does not remain in these simulations, an oxygen atmosphere could still be supported, especially for the higher end of the initial water range, and depending on assumed sinks. However, a dense O_2 atmosphere, with even a small amount of outgassed CO_2 , could produce an absorption feature at $15\mu\text{m}$ that is also precluded by the observational constraints ([Greene et al., 2023](#); [Ih et al., 2023](#); [Lincowski et al., 2023](#)). The tighter observational constraint that T1-b is currently desiccated and *also* likely does not have an oxygen atmosphere, combined with considerations of oxygen sinks over the lifetime of the system, will significantly lower this upper limit on initial water inventory.

Though detailed oxygen surface sink modeling is outside the scope of the current study, to give an example of how one may further constrain this upper limit we estimate a few oxygen sinks here, first considering only oxygen loss from the magma ocean and hydrodynamic escape while water loss is ongoing. Assuming magma ocean removal operates on the same timescales as hydrodynamic escape ([Hamano et al., 2013](#)), we estimate a removal of 3 TO of oxygen to the magma ocean (~ 630 bars on T1-b), based on studies of the early Venusian environment and theoretical studies on magma ocean evolution for the TRAPPIST-1 planets ([Barth et al., 2021](#); [Gillmann et al., 2009](#); [Schaefer et al., 2016](#); [Wordsworth et al., 2018](#)); and from our simulations we find 4 TO equivalents of oxygen would be lost to hydrodynamic drag. These combined give maximum initial surface water contents of 7 TO, to be consistent with an airless present day T1-b. However, loss of atmospheric oxygen can still continue after total loss of the water inventory, via processes such as non-thermal escape and dry crustal oxidation. Following [Krissansen-Totton & Fortney \(2022\)](#), we consider a non-thermal escape parameterization of ~ 100 bars of total oxygen loss across the system’s lifetime, and an average estimate of oxygen loss through dry crustal oxidation of ~ 10 Tmol/year (~ 55 bars/Gyr) after magma ocean solidification (following the perpetual runaway greenhouse scenario in [Krissansen-Totton et al., 2021b](#)). Given a system age of ~ 8 Gyr ([Birky et al., 2021](#)) and initial water contents of around 15 TO, T1-b may endure hydrodynamic escape for up to 1 Gyr, leaving 7 Gyr for dry crustal oxidation; thus, we conservatively estimate 385 bars of total oxygen removal through dry crustal oxidation. With these two additional oxygen sinks (magma ocean removal and dry crustal oxidation), our upper limit constraint on initial surface water, consistent with complete atmospheric erosion on T1-b at the present

day, would be lowered to 12 TO. However, note that with more rigorous modeling of oxygen removal, this upper limit would likely be higher. Overall we can conclude the upper limit on initial water content as constrained by observations of T1-b (Greene et al., 2023) is between 12 – 60 TO.

Although the above upper limit constraints on initial water abundance are developed with the observational constraint from TRAPPIST-1b, habitability studies of the system may be more concerned with the lower limit of initial water, which could inform the minimum amount of water the HZ planets possess at present-day. Constraining this lower limit may be possible by considering what we know of the atmospheric state of TRAPPIST-1c in addition to that of T1-b. Recent T1-c secondary eclipse observations with JWST/MIRI show a brightness temperature of $T_B = 380 \pm 31$ K (Zieba et al., 2023). This is 50K below, and $1.7\text{-}\sigma$ away from, the temperature expected for an airless body with zero heat redistribution (430 K). It is also $1.6\text{-}\sigma$ from an ultramafic surface with the strong weathering expected for this intensely UV-irradiated world (Zieba et al., 2023). The T1-c JWST $15\mu\text{m}$ data are best fit by either an airless world with a high albedo surface, or a thin <0.1 bar O_2 -dominated atmosphere (Lincowski et al., 2023; Zieba et al., 2023). However, other atmosphere types are still consistent with the data, including a 3 bar steam atmosphere, which is within $1.7\text{-}\sigma$ of the observed secondary eclipse value (Lincowski et al., 2023).

Given their different stellar distances, similar planetary properties and inferred geologic oxygen sinks, there is a narrow range of initial surface water contents that will simultaneously produce an airless T1-b and non-negligible oxygen on T1-c, even if both planets are found to be desiccated. As T1-b and T1-c are similarly interior to the HZ, possess comparable surface gravities ($g_{T1c} \sim 0.99g_{T1b}$), and likely formed with a similar composition ($\rho_{T1c} \sim 1.004\rho_{T1b}$) they likely experience comparable geologic and escape evolution. However, we have shown that since T1-c is slightly farther away from the host ($a_{T1c} \sim 1.37a_{T1b}$), it will retain more oxygen for equivalent amounts of water loss as T1-b due to the lower incident XUV flux (see §3.4 and Figure 3.7).

Considering oxygen removal through a magma ocean, dry crustal oxidation, and non-thermal escape, we run an Markov chain Monte Carlo (MCMC) to constrain the initial water content that would produce both an airless T1-b and a tenuous 0.1 bar O_2 -dominated atmosphere on T1-c, consistent with the currently available JWST data (Greene et al., 2023; Ih et al., 2023; Lincowski et al., 2023; Zieba et al., 2023). To conduct the MCMC, we use the publicly available **emcee** model (Foreman-Mackey et al., 2013). MCMC walkers fit for the initial water content by running VPlanet (Barnes et al., 2020) simulations of T1-b and T1-c that predict the oxygen build-up of the system. After a simulation, the estimated oxygen removal is subtracted, and the MCMC checks to see that T1-b has no oxygen remaining while T1-c is compared to a 0.1 bar oxygen atmosphere with an uncertainty of 10 bars, as a 10 bar oxygen atmosphere begins to show $>3\sigma$ disagreement from the $15\mu\text{m}$ measurement of T1-c (Zieba et al., 2023). As described earlier in the section, we estimate removal of 3 TO-worth of oxygen from a magma ocean (Barth et al., 2021; Gillmann et al., 2009), 100 bars from non-thermal escape (Krissansen-Totton & Fortney, 2022), and 10 Tmol/Gyr (~ 55 bars/Gyr) from dry crustal oxidation after the hydrodynamic escape period (Krissansen-Totton et al., 2021b). We vet convergence by considering the chain’s autocorrelation time; in total, we run 20 walkers for 80,000 steps with 1,000 burn-in steps (for a total of >1.5 million VPlanet simulations), this results in a chain length that is several times the autocorrelation time,

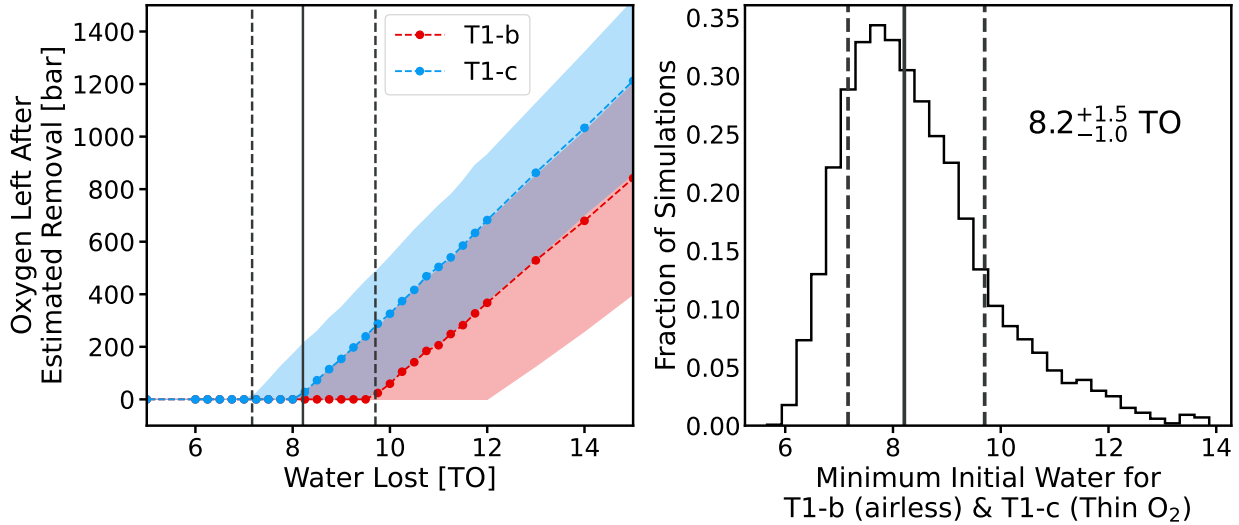


Figure 3.6: Left: The oxygen left in the atmospheres of T1-b (red) and T1-c (blue) after an estimated removal of 3 TO worth of oxygen from a magma ocean, 100 bars from non-thermal escape, and 10 Tmol/yr (~ 55 bars/Gyr) from dry crustal oxidation after the planet becomes desiccated (see text for estimation explanation). **Right:** The resulting histogram of initial water contents predicted by MCMC when fitting for the scenario that T1-b has lost all oxygen while T1-c retains 0.1 bar of atmospheric oxygen following the estimated removal. The vertical solid black lines on both panels denotes the 50th percentile value predicted by the MCMC while the vertical dashed black lines denote the 68% (1σ) confidence interval. This analysis predicts a minimum initial water content of $8.2^{+1.5}_{-1.0}$ TO to produce the desired final state, assuming both planets begin with the same initial water content. The amount of oxygen removal is meant to be an underestimate to produce a conservative lower limit, as additional oxygen removal would increase the minimum initial water required.

suggesting convergence has been achieved (Foreman-Mackey et al., 2013). We note that our oxygen removal parameterizations are meant to be low estimates of the total oxygen removal the planets may experience, as we are searching for a minimum initial surface water mass and greater oxygen removal would serve to raise the minimum.

Figure 3.6 shows the results of our MCMC analysis; the left panel is an illustration of the atmospheric oxygen left after removal by the estimated oxygen sinks, and the right panel is the distribution of initial water contents reported by the MCMC that best fit an airless T1-b and a T1-c with a 0.1 bar oxygen atmosphere. With 68% confidence (1σ) we find the minimum initial water content to be $8.2^{+1.5}_{-1.0}$ TO. This value with associated uncertainty is shown by vertical lines on both panels of figure 3.6.

As one last note, in considering the outer planets, under the assumptions of a similar magma ocean removal rate during hydrodynamic escape, followed by a removal of ~ 135 bars/Gyr analogous to geological O₂ sinks on the modern Earth (including weathering, volcanism, and subduction) (Catling, 2014), atmospheres lacking in O₂ are possible for all initial water contents considered. We point out, however, that these are rough estimates, and further work would be needed in tracking oxygen sinks over time to produce more accurate results.

3.4 Oxygen Retention Efficiency

Quantification of the oxygen retention efficiency allows us to evaluate the net balance between oxygen produced via water photodissociation and subsequent hydrogen escape, and oxygen loss due to drag during thermal hydrodynamic escape. Oxygen retention efficiency is given by:

$$\eta_{\text{Retention}} = \frac{M_{O_2, \text{produced}} - M_{O_2, \text{lost}}}{M_{O_2, \text{produced}}} \times 100, \quad (3.1)$$

where $M_{O_2, \text{produced}}$ is the total mass of oxygen that was produced by the cumulative hydrogen loss and $M_{O_2, \text{lost}}$ is the mass of oxygen that was lost through drag during escape. Note that this only takes into account production and losses via escape mechanisms, and oxygen may be further lost through sinks not considered here (e.g., Schaefer & Fegley, 2017; Schaefer et al., 2016).

Figure 3.7 shows the oxygen retention efficiency (Eq. 3.1) as a function of initial water content with contours for the 50th percentile values and 1 σ confidence region for all 7 planets. The color scale of Figure 3.7 shows, for a particular initial water content, the percentage of simulations that had a given oxygen retention efficiency. Additionally, Table 3.2 gives the 50th percentile values and 1 σ uncertainties for oxygen retention efficiency for our lowest (1 TO) and highest (500 TO) initial water case for all 7 planets. This result shows that oxygen retention efficiency increases with increasing orbital distance, initial water content, and planetary gravity. At low initial water contents, there is a strong distance dependence where efficiency increases with increasing orbital separation due to the drop in XUV flux; however, planets with low gravity may break this distance trend and show lower than expected O₂ retention efficiency when compared to the distance trend, such as T1-d and h. High initial water inventories (100 TO or more) typically lead to larger retention efficiencies than those for lower water inventories, and these retention efficiencies display a weaker distance dependence; for example T1-c at its largest initial water content possesses the largest retention efficiency of any planet. This is because high initial water contents sustain escape to much later ages; as oxygen loss through drag will be higher early on with a higher XUV environment, decreasing with time as XUV decreases, the cumulative oxygen retention efficiency will be higher for planets that remain in active escape to later times. In comparison, planets where hydrodynamic escape shuts off earlier will have lower cumulative oxygen retention efficiency because all loss processes occur in a high XUV environment. This influence is further shown by the plateau of retention efficiency as planets reach initial water contents that lead to their maximum possible water loss (i.e., the maximum amount of water they may lose given the maximum possible simulation time and an effectively infinite initial reservoir), indicating that retention efficiency is directly dependent on time spent in the escape regime with evolving XUV conditions, which is in turn dependent on initial water. At low initial water contents, the interior planets (T1-b, c, and d) retain $\sim 10\% - 30\%$ of oxygen produced, while the outer planets retain $\sim 40\% - 70\%$. At high initial water contents, this number increases to $\sim 70\% - 90\%$ for all planets in the system, excluding T1-h, which has extremely low gravity and loses $\lesssim 1$ TO for any initial content, thus displaying retention efficiency that remains at $\sim 46\%$ even as initial water increases.

However, counter to the general trend of retention efficiency increasing with initial water

content described above, we also find that there is a limited range of initial water contents for each planet where feedback from diffusion processes causes retention efficiency to *decrease* with increasing initial water; this decreasing behavior is particularly noticeable for T1-d near ~ 100 TO and T1-e near ~ 10 TO in Figure 3.7. For a particular planet, this decreasing behavior occurs when the initial water content approaches an amount large enough to prevent the planet from entering the diffusion-limited escape regime over its escape lifetime (either prior to entering the HZ, or up to present day). Since diffusion-limited escape prohibits oxygen loss and favors oxygen retention, avoiding a diffusion-limited escape period will decrease oxygen retention efficiency. Thus, when this regime is prevented entirely, we see a range where retention efficiency decreases with increasing initial water, as the influence of the lack of diffusion-limited escape outweighs the gain in efficiency from increasing the mixing ratio of water. However, this behavior only occurs for a narrow range of initial water abundances, and increasing efficiency with increasing initial water contents is seen on either side of that range.

When losing equal amounts of water a strong distance dependence persists of increasing retention efficiency with increasing orbital distance, even when increasing initial water content; this behavior is apparent by the results in Table 3.3, which show the efficiency of oxygen retention following an equal loss of 1 TO for a low (1 TO) and high (9, 10, or 11 TO) initial water case. Note, as this result compares an equal water loss, simulations that do not lose a full TO are not included. Consequently many cases for T1-g, and all cases for T1-h are excluded, as the former does not typically lose a full TO when it has a low starting inventory, and the latter does not typically lose a full TO for any starting inventory considered. Overall, decreases in orbital distance, initial water, and gravity will all decrease oxygen retention efficiency.

Oxygen Retention Efficiency [%] for Cumulative Water Loss		
Body	Lowest Initial, 1 TO	Highest Initial, 500 TO
T1-b	$9.979^{+21.39}_{-9.725}$	$81.11^{+4.999}_{-5.410}$
T1-c	$32.79^{+15.35}_{-21.01}$	$89.14^{+4.122}_{-4.221}$
T1-d	$11.11^{+10.74}_{-7.668}$	$68.71^{+6.393}_{-6.157}$
T1-e	$42.31^{+12.24}_{-13.17}$	$70.68^{+9.078}_{-9.853}$
T1-f	$64.78^{+9.762}_{-10.98}$	$81.04^{+7.487}_{-8.562}$
T1-g	$76.14^{+7.546}_{-9.347}$	$86.43^{+6.227}_{-7.829}$
T1-h	$38.13^{+13.12}_{-10.76}$	$46.87^{+10.72}_{-9.938}$

Table 3.2: The efficiency of oxygen retention [%] after the cumulative water loss predicted by our model at the lowest (1 TO, middle column) and the highest (500 TO, right column) initial water content. Uncertainties reported are 1σ .

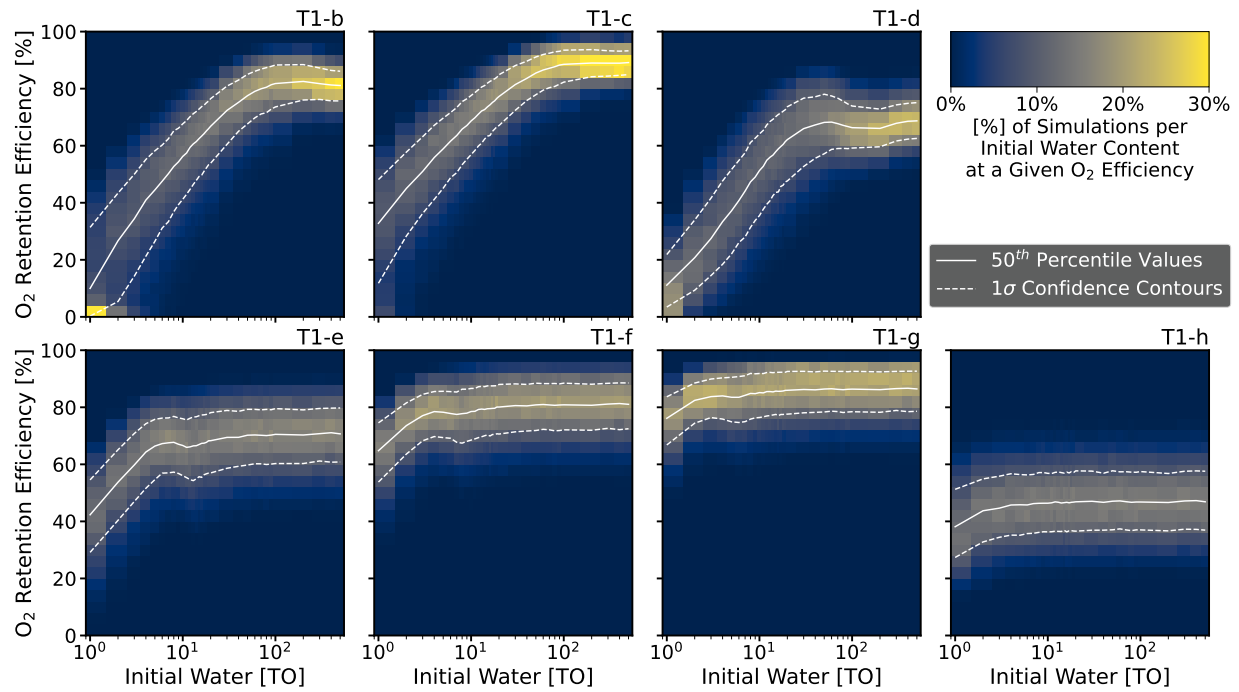


Figure 3.7: Oxygen retention efficiency as a function of initial water content in TO. **Top Row:** Interior planets, T1-b, c, and d. **Bottom Row:** Outer planets, T1-e, f, g, and h. Coloring shows the percentage of simulations at a particular initial water content that fell in a given oxygen retention efficiency bin (e.g., each column corresponds to one initial water content and sums to 100%). Contours are given for the 50th percentile values (solid white lines) and the 1 σ confidence region (dashed white lines).

Oxygen Retention Efficiency [%] for a 1 TO Loss		
Body	Initial 1 TO	Initial 9, 10, or 11 TO
T1-b	$9.979^{+21.39}_{-9.725}$	$16.83^{+14.31}_{-8.395}$
T1-c	$32.79^{+15.35}_{-21.01}$	$32.85^{+11.90}_{-15.40}$
T1-d	$11.11^{+10.74}_{-7.668}$	$17.49^{+6.754}_{-6.181}$
T1-e	$42.31^{+12.24}_{-13.17}$	$39.49^{+10.33}_{-9.698}$
T1-f	$64.78^{+9.762}_{-10.98}$	$60.31^{+10.46}_{-10.87}$
T1-g	—	$73.12^{+9.158}_{-10.69}$
T1-h	—	—

Table 3.3: The efficiency of oxygen retention [%] following a 1 TO water loss. Uncertainties reported are 1σ . The middle column shows the results for planets with an initial inventory of 1 TO, and the right column shows the results for planets with an initial inventory of 9, 10, or 11 TO.

3.5 Comparison to Atmosphere-Interior Evolution Model

Here we compare our calculated escape rates to [Krissansen-Totton & Fortney \(2022\)](#), a similar study modeling the atmospheric evolution of the TRAPPIST-1 planets, but with a particular focus on the interior evolution and surface-atmosphere exchange. [Krissansen-Totton & Fortney \(2022\)](#) use the Planetary Atmosphere, Crust, and MANTle (PACMAN) evolutionary model to simulate terrestrial planet mantle and atmosphere evolution from an initial magma ocean phase through solidification to temperate geochemical cycling on the TRAPPIST-1 planets (validated in [Krissansen-Totton et al., 2021a,b](#)). They complete 5000 model runs total for each planet; unlike this study, their simulations sample initial water in log space from 0.7 – 300 TO. For the interior planets, T1-b, c, and d, they show half of all model runs produce >1 bar oxygen atmospheres while the other half result in airless bodies. Alike to the current study, oxygen-rich modern atmospheres become less probable as distance from the star increases, noting that while initial water has the largest effect on oxygen build-up for the inner planets, atmospheric escape physics and geological factors influence the outer planets more heavily. Overall, [Krissansen-Totton & Fortney \(2022\)](#) show that complete atmospheric erosion or oxygen-rich atmospheres are most likely for the inner planets, while the outer planets are more likely to possess CO_2 or CO_2/O_2 dominated atmospheres, the latter occurring if CO_2 efficiently acts as a secondary producer of oxygen through photodissociation.

Figure 3.8 shows a comparison of the rates of H_2O loss and oxygen build-up with 2σ uncertainty envelopes, as presented in [Krissansen-Totton & Fortney \(2022\)](#), with our work for T1-b, an interior planet, and T1 e, a HZ planet. Both studies adopt the stellar evolution models of [Baraffe et al. \(2015\)](#), and XUV properties from [Birky et al. \(2021\)](#), meaning

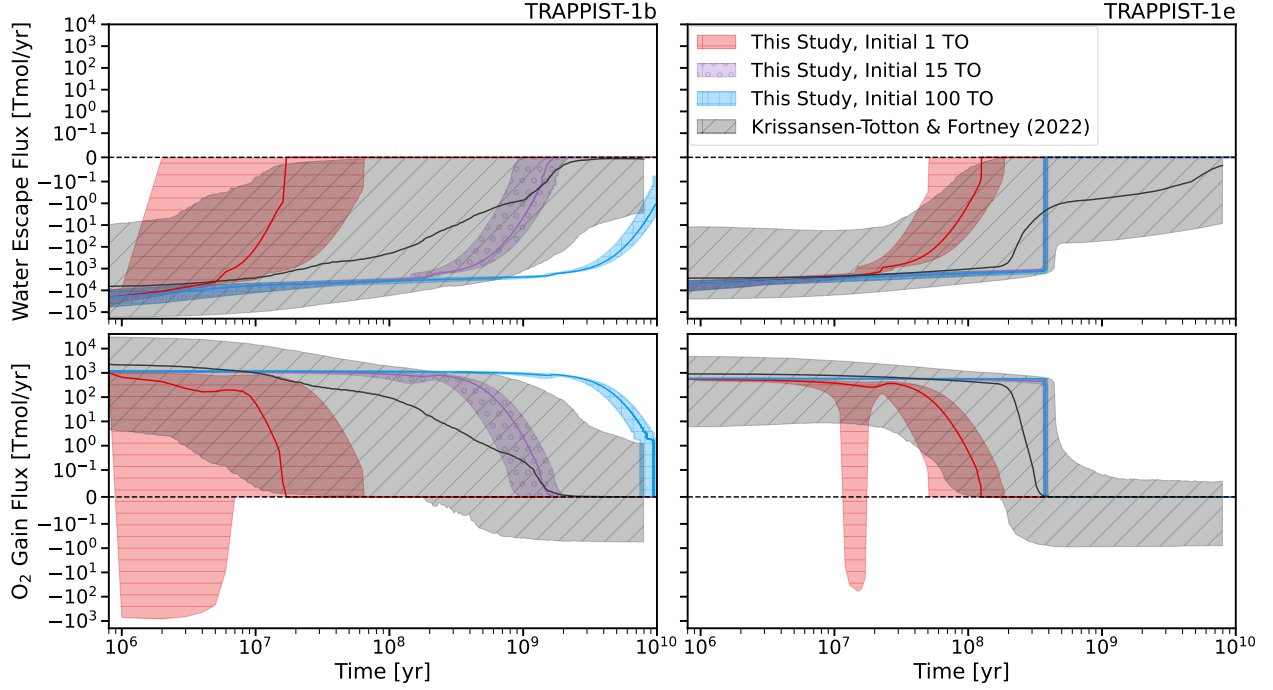


Figure 3.8: A comparison of the water loss and oxygen production rates from Krissansen-Totton & Fortney (2022) to this study. Design of the figure is meant to recreate the style published in Krissansen-Totton & Fortney (2022); all shaded regions denote 2σ uncertainties. The red, purple, and blue lines and shaded regions show the results from this study for initial water contents of 1, 15, and 100 TO, respectively, and the grey line and shaded region shows the results presented in Krissansen-Totton & Fortney (2022). **Left Column:** Comparisons for the interior planet TRAPPIST-1 b (see Figure 2 in Krissansen-Totton & Fortney, 2022). **Right Column:** Comparisons for the habitable zone planet TRAPPIST-1 e (see Figure 3 in Krissansen-Totton & Fortney, 2022). **Top Row:** Rate of water loss due to thermal atmospheric escape [Tmol/yr] over time in years. Note, as water is being lost, the flux is negative. **Bottom Row:** Rates of oxygen production (i.e., gain flux) [Tmol/yr] due to water photolysis and subsequent hydrogen escape over time in years. In general, our results are in agreement with those of Krissansen-Totton & Fortney (2022), and our median test case with an initial water inventory of 15 TO (log space average between 0.7 and 300 TO) stays within their model uncertainties for the entire age of the system. Note, in the T1-e comparisons, our 15 and 100 TO cases display nearly identical evolution and overlap on the plot.

differences in our work are not due to dissimilar XUV environments. Since we consider initial water contents on a grid, rather than the randomly sampled input of Krissansen-Totton & Fortney (2022), we compare 3 of our initial water contents in Figure 3.8; we show initial contents of 1 and 100 TO to bracket the median water contents from Krissansen-Totton & Fortney (2022), and an initial content of 15 TO is shown as the average value of 0.7 and 300 TO in log space.

The agreement between our studies is favorable, with our median 15 TO case remaining within the 2σ uncertainty region of Krissansen-Totton & Fortney (2022). The average rates from Krissansen-Totton & Fortney (2022) and from all shown initial water contents in this study begin in near perfect agreement ($\lesssim 10^7$ years), with our 1 TO case deviating first as desiccation is reached quickly. For T1-b, our 100 TO case begins to deviate more at ~ 1 Gyr, showing relatively larger fluxes of both water escape and O_2 production as more water is available to sustain escape than the majority of model runs from Krissansen-Totton & Fortney (2022). Our 15 TO T1-b case remains in close agreement for the entirety of the system’s lifetime, although the shape of the curves show that escape rates in Krissansen-Totton & Fortney (2022) slow more gradually. For T1-e, entrance to the HZ strictly ends evolution for our 15 and 100 TO cases at ~ 380 Myr. However, as Krissansen-Totton & Fortney (2022) did not use as stringent of a simulation halt, they still report minor water loss and oxygen production past this point, although it is significantly reduced. Before HZ entrance, our 15 and 100 TO T1-e cases behave similarly, but the 15 TO case does begin to deviate and show more quickly lowering rates suggesting it would remain in better agreement with Krissansen-Totton & Fortney (2022), as expected. In general, 2σ uncertainties on the results shown in this study are smaller because the curves each have a fixed initial water content, while random sampling of initial water content in Krissansen-Totton & Fortney (2022) contributed to larger uncertainty in simulation behavior.

When oxygen drag is efficient, a “negative gain flux” may occur, where oxygen is lost faster than it is photolytically produced, which could deplete existing atmospheric oxygen inventories. Figure 3.8 shows these negative O_2 gain fluxes early in the age of the system ($\lesssim 200$ Myr), which we were only able to reproduce with VPLanet after the model modifications implemented here. We found that closer-in planets with lower initial water contents are more likely to experience a negative O_2 gain flux. For example, with an initial water content of 1 TO for T1-b and T1-e, 62% of the T1-b and 35% of the T1-e simulations experienced at least one time step with a negative O_2 gain flux, respectively; this number dropped to 16% and 4%, respectively, when initial water was increased to 2 TO.

Negative O_2 gain fluxes occur when the mixing ratio of oxygen is as high as possible without pushing escape into the diffusion-limited regime, and must occur during periods of high incident XUV (e.g., $\lesssim 200$ Myr). As the mixing ratio of oxygen increases, loss to hydrodynamic drag also increases (e.g., Eq. 2.9); but if the mixing ratio of O_2 exceeds that of water, the atmosphere will enter diffusion-limited escape and oxygen drag will be shut-off altogether. Negative O_2 gain flux is therefore most likely to occur during periods when the incident XUV is high (e.g., $\lesssim 200$ Myr), and when the mixing ratio of oxygen approaches the maximum value needed to trigger diffusion limited escape and the shut down of oxygen drag. A negative O_2 gain flux will then continue until diffusion-limited escape starts or the XUV flux has decreased sufficiently. Considering our 1 TO cases in Figure 3.8, T1-b starts to lose net atmospheric O_2 almost immediately due to its close proximity to the star, whereas T1-e

needs at least 10 Myr to enter a negative O_2 gain flux state, as some time is needed for the oxygen mixing ratio to increase sufficiently.

4 Discussion

We have used the most recently available constraints on the TRAPPIST-1 system (Agol et al., 2021; Birky et al., 2021) and a hydrodynamic atmospheric escape model to statistically explore the ranges of possible water loss and oxygen buildup on the TRAPPIST-1 planets. Improving on past studies, we combine observational uncertainties on the stellar luminosity evolution and planetary parameters to construct self-consistent input chains that are randomly sampled for each simulation, fully incorporating the statistically plausible region of initial conditions for physical system parameters. Without considering outgassing, we find the interior planets (T1-b, c, and d) nearly, or completely, lose all of their initial surface water for all but the largest initial contents (when initial water is $>50 - 100$ TO), while the outer planets (T1-e, f, g, and h) only become desiccated for the very lowest initial water contents considered ($1 - 2$ TO). Given that our model halts hydrodynamic escape when a planet enters the habitable zone, the outer planets never lose more than 10 TO total, which results in maximum possible oxygen retention values spanning $\sim 90 - 1290$ bars. Comparing our results on planetary water loss and oxygen production rates to those reported in Krissansen-Totton & Fortney (2022), we find that rates from an example set of 3 of our tested initial water contents remained within their reported uncertainties for most, or the entirety, of the age of the system, showing favorable agreement.

We find that atmospheric oxygen retention – what fraction of the oxygen produced by water photolysis is retained in the atmosphere – is a function of both planet-star separation and initial water inventory. Closer to the host star, we find that larger percentages of photolysis-produced oxygen are lost due to hydrodynamic drag, offsetting the substantial oxygen produced by water photolysis. For the cumulative water loss at low initial contents, our simulations show that the interior planets (T1-b, c, and d) retain $\sim 10\% - 30\%$ of the oxygen generated, and the outer planets (T1-e, f, and g) retain $\sim 50\% - 70\%$. At high initial water contents, this retention efficiency approaches $\sim 70\% - 90\%$ for all planets in the system, excluding T1-h. However, despite the enhanced loss rate of oxygen, for initial water contents of more than 4-5 TO, the overall production rate is sufficiently high that the interior planets always retain more O_2 than the outer planets. Consequently, for initial water contents $\lesssim 4$ TO, the outer planets are more likely to retain atmospheric oxygen.

We retrieved the suite of plausible water evolutionary histories consistent with a known or predicted final water mass fraction (WMF) for the outer planets, demonstrating a mechanism to determine the most probable initial water content of the planet for a predicted final water content. For the maximum present-day WMFs constrained by measured planetary densities Agol et al. (2021), we find the most probable initial water contents for all outer planets to be in the range of $\sim 80 - 300$ TO. For T1-e, we interpolated from this probability data to report the 1σ confidence interval on our maximum initial water content prediction of $90.6^{+70.6}_{-37.2}$ TO, based on the model we employ and the present-day water constraints we adopt. This analysis is a proof of concept for a method to retrieve probable initial water content from an assumed present-day state. However, our model assumptions will produce upper limits, and the true

initial water content may be much lower, as we assume that 1) the planets' low densities are entirely due to their WMF, and 2) that water was not sequestered in the planetary interior, but was always on the surface and accessible to atmospheric loss. To elaborate on the latter point, if water was instead partially or fully trapped in the planetary interior, less initial water would be required to recreate the same WMF at present-day, as it would be protected from loss due to escape.

4.1 Behavior of Water Loss

Our work shows that water loss rates and cumulative water lost are highly dependent on the incident XUV flux and the atmospheric mixing ratio of water; implying both orbital distance and initial water content exert strong influence on the end state observed. Qualitatively, increasing orbital distance will decrease water loss by decreasing incident XUV, and decreasing the time to HZ entry and hydrodynamic escape shutoff. Conversely, increasing initial water content will increase water loss rates by creating a higher atmospheric water mixing ratio at earlier ages during greater incident XUV. Across the conditions considered in this work, the interior planets (T1-b, c and d) frequently lose their entire initial water inventory, while the outer planets (T1-e, f, g and h) are more likely to retain water to the present-day.

As the interior planets are located close enough to the star to experience escape for the entirety of the system's lifetime, their end state is most heavily influenced by initial water content (see Figure 3.1), which is in agreement with (Krissansen-Totton & Fortney, 2022). Conversely, the end state behavior of the HZ or outer planets (T1-e, f, g, and h) is primarily influenced by distance from the host star, which affects total integrated XUV flux experienced by the planet, and also determines the time to habitable zone entrance (i.e., total time spent in the hydrodynamic escape regime). For the outer planets, escape is shut off at HZ entrance due to the assumed formation of a cold trap; however, we caution that the true efficacy of a cold trap to prevent hydrodynamic escape may not be this efficient, and may be influenced by other factors (see also §4.4). As HZ entrance results in a short period of escape ($\sim 50 - 400$ Myr) relative to the age of the system ($\tau \sim 8$ Gyr) for the outer planets, desiccation is rarely witnessed and the maximum amount of water they may lose through hydrodynamic escape is <10 TO in all cases in this study, and as low as 0.8 TO for T1-h. Though the outer planets may better constrain initial water content when considering measurements of present-day WMF, measuring the present-day WMF is observationally challenging as water may be sequestered in the interior or in a surface ocean, and so not amenable to transmission observations, and also difficult to derive uniquely from planetary density constraints (Agol et al., 2021). However, initial water more heavily influences the present-day atmospheric oxygen abundance on the interior planets, and ocean-loss generated O_2 , or its proxy O_3 , may be accessible in JWST observations (e.g., Lustig-Yaeger et al., 2019a) and next generation ground-based telescopes (e.g., Currie et al., 2023), and so may provide the first strong constraints on the initial water content of the planetary system as a whole, when considering current and near-term observational capabilities.

4.1.1 Comparison with Previous Work

Comparison with past studies shows agreement in our predictions that the inner planets are more likely to be desiccated, but the outer planets retain water, and that stellar XUV and activity evolution have larger impacts on total water loss than geological processes. Our results confirm numerous past studies that desiccation is possible on the interior planets of TRAPPIST-1, or a similar M dwarf system, for all but extremely large initial water contents (Bolmont et al., 2017; Bourrier et al., 2017b; Johnstone, 2020; Krissansen-Totton & Fortney, 2022; Luger & Barnes, 2015; Schaefer et al., 2016). Similarly, we also find maximum water loss on the HZ and outer planets of $\sim 1 - 10$ TO, implying these planets may still possess water at present-day (Barth et al., 2021; Bolmont et al., 2017; Bourrier et al., 2017b; Krissansen-Totton & Fortney, 2022; Luger & Barnes, 2015). Comparison with past studies shows that predicted water loss is very sensitive to assumptions on the stellar XUV and activity evolution, implying that tighter constraints on TRAPPIST-1’s stellar spectrum and activity can greatly improve predictions for planetary outcomes. For example, Bolmont et al. (2017) (considering T-1b and c) and Bourrier et al. (2017b) (considering all 7 planets in the system) adopt XUV saturation fractions $\sim 1.32\times$ and $\sim 2.5 - 3.5\times$ smaller than this work, respectively. Consequently, water loss predictions for the inner planets in this study are up to $3\times$ larger than Bolmont et al. (2017) and $>3\times$ larger than Bourrier et al. (2017b). Comparison of our results, which do not include geological processes, with those of Krissansen-Totton & Fortney (2022), that do, suggest that the inclusion of geologic processes (e.g., sequestration of water in the planetary interior and outgassing over time) has less of an influence on total water loss than changing XUV environment, since Krissansen-Totton & Fortney (2022) adopts the same XUV parameterizations (Birky et al., 2021) as this study and reports agreement on overall conclusions on the final planetary water contents. These comparisons highlight how marginal increases in XUV flux may produce drastic increases in water loss, and suggest more observations of the TRAPPIST-1 stellar environment may translate to significant improvements in model predictions.

4.2 Oxygen Production, Retention and Loss

The upper limits on oxygen production and retention quantified by this study provide important environmental context on atmospheric O_2 in the TRAPPIST-1 system, and while retained atmospheres less than 1 bar may constitute a false positive for an O_2 biosignature (Meadows, 2017; Schaefer et al., 2016), significantly larger amounts may be a clear indication of an abiotic post-ocean loss atmosphere (Luger & Barnes, 2015). On Earth-sized terrestrials, the loss of an ocean’s worth of water will generate ~ 250 bars of O_2 , and the inner planets, which lose more water over the system lifetime, can produce hundreds to thousands of bars atmospheric oxygen, depending on initial water content. However, not all this oxygen is retained, and significant losses can occur due to energetic hydrogen escape flows that remove the oxygen from the atmosphere. We find that cumulative oxygen retention increases with increasing distance from the star; however, for initial water contents greater than $4 - 5$ TO, the interior planets retain more oxygen cumulatively than the outer planets due to greater overall water loss (and the subsequent increase in oxygen production).

Similarly, we find the efficiency of oxygen retention increases with increasing distance from

the star and/or increasing initial water content (§3.4, Figure 3.7). The distance dependence is due to greater XUV flux at small orbital separations, resulting in more energetic escape flows and oxygen loss through drag; however, planets with low gravity, including T1-d and h, may deviate from this pattern and lose more oxygen than their closer-in neighbors. The increase in the efficiency of oxygen retention with increasing initial water content is driven by larger water inventories producing a large atmospheric water to oxygen ratio, which decreases the rate of oxygen loss through drag.

Low oxygen retention efficiencies are also more likely to occur when oxygen mixing ratios are higher, but before the oxygen fraction exceeds the water fraction in the atmosphere, triggering diffusion limited escape and oxygen retention. Extremely low initial water contents can lead to high oxygen mixing ratios early in the system’s lifetime, during the greatest incident XUV, resulting in highly efficient oxygen drag and lowered retention efficiency – in some cases leading to total oxygen loss and atmospheric erosion for the interior planets. A similarly lowered retention efficiency could also occur if the initial planetary water inventory was high, but sequestered in the interior and slowly outgassed, rather than being continuously available for escape at the surface as is often assumed (e.g., [Krissansen-Totton & Fortney, 2022](#)). In this case, the throttling of the water availability by outgassing would be more likely to result in lower atmospheric water mixing ratios at any given time leading to greater oxygen loss through drag.

4.2.1 Comparison with Previous Work

In contrast to the general agreement on water loss predictions we see across previous studies (§4.1.1), predictions of oxygen retention for M dwarf planets vary. In this work, we witness a broad range of oxygen retention scenarios depending primarily on initial water content and orbital distance. For medium to high initial water inventories (typically above ~ 5 TO) we predict comparatively high planetary oxygen retention (e.g., hundreds to thousands of bars), which is in agreement with several previous studies ([Bolmont et al., 2017](#); [Bourrier et al., 2017b](#); [Krissansen-Totton & Fortney, 2022](#); [Luger & Barnes, 2015](#)). In contrast, others show that little to no oxygen would survive hydrodynamic escape processes (e.g. zero to tens of bars) even at medium to high initial water contents ([Johnstone, 2020](#); [Schaefer et al., 2016](#)). Within these predictions, there is further disagreement as to the precise quantity of oxygen retained, and if it would remain in the atmosphere (e.g., [Luger & Barnes, 2015](#)) or be removed partially or entirely by reactions with iron in the planet’s mantle (e.g., [Barth et al., 2021](#); [Krissansen-Totton & Fortney, 2022](#); [Wordsworth et al., 2018](#)).

At low water contents ($\lesssim 4$ TO), this work indicates that large percentages, or even the entirety of photolytically produced oxygen may be lost solely through drag during hydrodynamic escape (as demonstrated in Figures 3.3, 3.7, and 3.8); similar results with complete oxygen loss have been reported by several previous studies ([Johnstone, 2020](#); [Krissansen-Totton & Fortney, 2022](#); [Schaefer et al., 2016](#)). [Schaefer et al. \(2016\)](#) considers water contents up to 1000 TO in the GJ 1132 system ($M_* = 0.181 M_\odot$, see [Berta-Thompson et al., 2015](#)) and show that the super-Earth GJ 1132 b would likely lose 90 – 99% of all photolytically produced oxygen to space through drag. Likewise, the [Schaefer et al. \(2016\)](#) model was also adopted by [Kreidberg et al. \(2019\)](#) which reported that initial water contents < 240 TO resulted in complete atmospheric loss on LHS 3488 b. Comparing GJ 1132 b and LHS 3488

b to T1-b in the TRAPPIST-1 system, they have substantially larger insolation – with GJ 1132 b receiving about 19 times more flux than Earth (Schaefer et al., 2016) and LHS 3488 b receiving 70 times more flux than Earth (Vanderspek et al., 2019), whereas T1-b receives only about 4 times more than Earth (Agol et al., 2021). This higher incident radiation helps to explain why such high oxygen loss rates are reported. Similar oxygen behavior was shown by Johnstone (2020) when considering an Earth-like planet with an M dwarf host, reporting water loss up to 120 TO during the stellar saturation time (the first 1 Gyr) with little to no planetary oxygen retention as a result of efficient drag. However, when considering medium to high initial water contents ($>4 - 5$ TO) and also accounting for drag, our results instead predict a significant build-up of oxygen. This contradicts the work of Johnstone (2020), but is consistent with several other studies, which predict oxygen build-up ranging from several hundreds (Bolmont et al., 2017) to thousands of bars (Luger & Barnes, 2015) on the interior planets, and several tens (Bolmont et al., 2017) to hundreds of bars (Barth et al., 2021; Luger & Barnes, 2015) on the outer planets. These differences in predictions are likely because, as we have shown, the precise amount of build-up is highly dependent on duration of escape, planetary gravity, and mathematical descriptions of crossover mass and oxygen flux. Observations to constrain atmospheric oxygen on the TRAPPIST-1 planets would help constrain evolutionary scenarios and outcomes, and improve theoretical models.

4.3 Constraining the Early Water Abundance of the TRAPPIST-1 Planets

We explore the process of constraining initial water content of the TRAPPIST-1 planets, both through model inference (§3.3.1) and by considering recent JWST measurements. By combining simulations and JWST data from multiple planets – in this case, TRAPPIST-1 b and c – we can derive much tighter constraints on initial surface water abundance (§3.3.2).

4.3.1 Statistically Retrieving Planetary Initial Water Content

As we show in Section 3.3.1, given present-day water and oxygen inventories, our model suite of escape histories can provide statistical constraints on initial water content and past water loss. While using constraints on present day water inventories informed by measured planetary densities can provide a key constraint (Agol et al., 2021), future observational evidence on the presence and nature of the TRAPPIST-1 atmospheres could be used to refine initial water content and subsequent planetary evolution. For example, if an outer planet is found to be desiccated, it would place a strict upper limit on initial water content, given the much shorter escape lifetimes for outer planets. Correspondingly, desiccation on an interior planet provides weaker constraints as there is a much broader range of initial water abundances that could still result in desiccation over the system lifetime (§4.3.2). For a desiccated interior planet, oxygen may be a better indicator of ocean loss and other evolutionary processes as it is much more tightly correlated to initial water content (see Figure 3.2). If a planet is observed to still possess water, the method explored in Section 3.3.1 and Appendix 7.1 demonstrates a basic framework for conducting statistical inference to achieve an initial upper limit constraint on initial water.

Statistical inference may also be leveraged as a model intercomparison tool, and to provide critical constraints on planet formation, migration and water delivery models. In the example of the current work, if multiple studies on water loss conduct an analysis to map initial to final water content, we can indirectly compare the latent space (e.g., exact equations, order of operations, timestepping, etc) predicted by those models during evolution. In a more concrete sense, our method of retrieving initial from final water content applied to the TRAPPIST-1 system can provide model constraints for formation and water delivery scenarios of the system. Even with relatively uncertain constraints on initial water content, this may inform if the planets formed *in situ* or past the snow line followed by inwards migration (Raymond et al., 2022).

4.3.2 Combining JWST Observations of T1-b & T1-c to Further Constrain Initial Water Inventory

Recent observations of TRAPPIST-1b and c have demonstrated that the former may be an airless world (Greene et al., 2023; Ih et al., 2023), while the latter may be better fit by a tenuous oxygen-dominated atmosphere (Lincowski et al., 2023; Zieba et al., 2023). In Section 3.3.2, we used MCMC to fit for the initial water content that would produce this final atmospheric state when assuming basic oxygen sink estimations and that the two planets formed with comparable water inventories; the results of this analysis are shown in Figure 3.6. Our MCMC reported that the minimum initial water content of the planets is $8.2^{+1.5}_{-1.0}$ TO. This estimated range is in agreement with Zieba et al. (2023), who suggest an initial water mass of $9.5^{+7.5}_{-2.3}$ TO through an analysis of conservative CO₂ upper limit constraints, albeit with a similar atmospheric escape model (Luger & Barnes, 2015; Schaefer et al., 2016).

These constraints on minimum initial water using JWST observations of T1-b and c, and our estimates of subsequent water and oxygen escape and loss, have important ramifications for the presence of water, and habitable conditions, on the TRAPPIST-1 habitable zone planets. If all planets in the system formed with comparable initial water contents, as supported by the delicate resonance chain and recent formation studies (e.g., Raymond et al., 2022), our simulations suggest that an initial water content of 8 TO would imply the HZ and outer planets would still possess water after escape is shut off upon entrance to the habitable zone. With an initial water content of 8 TO, we find T1-e, f, g, and h would possess $1.7^{+0.47}_{-0.57}$, $3.6^{+0.32}_{-0.46}$, $4.8^{+0.21}_{-0.29}$, and $7.2^{+0.14}_{-0.20}$ TO, respectively, after HZ entrance. Thus, a confirmation of oxygen in the atmosphere of T1-c would increase the probability that the HZ planets retained water and could be potentially habitable.

If T1-c is airless or nearly airless, this still may provide information on an upper limit on initial water of the system, for example this would narrow our previous upper limit constraint from T1-b alone; following the same removal estimates described in section 3.3.2, we find an airless T1-c would suggest an upper limit on initial surface water of 9 TO. Alternatively, in this airless T1-c scenario, Zieba et al. (2023) predict initial water content would be reduced to ~ 4 TO; for this initial water, our model predicts T1-e, f, g, and h would possess $0.03^{+0.05}_{-0.03}$, $0.52^{+0.15}_{-0.17}$, $1.2^{+0.14}_{-0.19}$, and $3.22^{+0.14}_{-0.20}$ TO, respectively, after HZ entrance. Although this case would imply a greater risk of water loss on T1-e and f, it would not rule out surface water on these planets and would still support considerable endowments on T1-g and h. This is in agreement with the conclusion of Krissansen-Totton (2023) that an airless T1-b (and c)

does not preclude the outer planets from possessing substantial atmospheres.

If the TRAPPIST-1 HZ and outer planets are likely to possess present-day oceans, as the recent JWST observations (Greene et al., 2023; Zieba et al., 2023) interpreted with our models suggest, then these will make important targets for JWST observations. When observing these targets in transmission, however, the further work will be required to remove the effects of stellar contamination from the data, as recent observations have shown to be prevalent (Lim et al., 2023; Rackham et al., 2018). Though O_2 has been shown to be extremely difficult to detect with JWST, particularly for the outer planets, which will be restricted to transmission measurements (e.g., Gialluca et al., 2021, 2023; Lustig-Yaeger et al., 2019a; Meadows et al., 2023; Wunderlich et al., 2019), post-ocean loss O_2 atmospheres may be detectable on the interior planets by using secondary eclipse MIRI observations to search for the O_3 that is produced by O_2 photolysis.

4.4 Broader Planetary Environment & Model Limitations

Future changes to our understanding of initial conditions, model treatment of escape, and the planetary environment post-hydrodynamic loss may influence our results, and we discuss potential ramifications here. Several changes within the model itself may create a more realistic treatment of the escape process, most notable of which would be the addition of a defined atmospheric vertical structure and variable pressure-temperature profile, and the inclusion of non-thermal escape; these beneficial model changes are discussed in Section 4.4.1. In the current study we have explored a broad range of initial water contents at a fixed escape onset time of 1 Myr; however, formation and water delivery research on the TRAPPIST-1 system may provide valuable information that would allow us to narrow the allowed range of initial water contents and conserve computational expense – these considerations are discussed in Section 4.4.2. All of these considerations should be kept in mind when using this work to interpret observations of the system.

4.4.1 Beneficial Model Changes & Additions

Several model updates would make our treatment of the hydrodynamic escape period more realistic, and we find the overwhelming majority of which would likely serve to reduce the cumulative water loss, suggesting the results presented in this study are upper limits to water loss and oxygen accumulation. Since our simulations currently assume atmospheres with perfect mixing and constant pressure and temperature, approximations in escape physics are required as vertical transport and temperature gradients are neglected. Approximations commonly made in escape modeling (Bourrier et al., 2017b; Luger & Barnes, 2015; Schaefer et al., 2016; Tian, 2015) may over- or under-estimate loss rates, particularly in the energy-limited formalism (Krenn et al., 2021) or at boundary conditions between escape regime changes (Gronoff et al., 2020; Volkov et al., 2011). Our description of hydrodynamic escape follows the energy-limited approximation (Hunten, 1973; Watson et al., 1981) however, it has been shown that this formalism may considerably deviate from hydrodynamic mass loss models in certain scenarios. Based on Krenn et al. (2021), which assesses the scenarios in which the energy-limited approximation is applicable, all the planets in our study remain in agreement with the more rigorous hydrodynamic loss simulations of Krenn et al. (2021)

within a factor of 10 for the entirety of our simulations, except T1-d, and h, and T1-e at the end of their simulations.

Other escape processes not considered in this work may also be acting upon the atmosphere, such as non-thermal escape (e.g., [Dong et al., 2018](#)), photochemical escape (e.g., [Wordsworth et al., 2018](#)), and core-powered mass-loss (e.g., [Ginzburg et al., 2016](#); [Gupta & Schlichting, 2019](#)). Though in the case of core-powered mass-loss, this is more typically explored for super-Earth and sub-Neptune populations, and will likely have a greater effect on an initial H/He envelope ([Gupta & Schlichting, 2019](#)) which we did not take into consideration in this work.

In this work, no photochemistry besides photolysis, and no geological evolution or surface-atmosphere exchange was modeled. In reality, photochemical reactions play a pivotal role in atmospheric escape, particularly in UV shielding, the creation of photochemical products that may act as UV shields, and effects on atmospheric heating and cooling. Through UV shielding, particles at higher altitudes may absorb UV radiation and protect molecules lower in the atmosphere from photodissociation, including self-shielding (e.g., O₂ protecting other O₂ molecules) and shielding between molecular species ([Calahan et al., 2022](#)). Of notable importance, the absorption cross sections of water, O₂, O₃, and CO₂ overlap heavily ([Domagal-Goldman et al., 2014](#); [Parkinson & Yoshino, 2003](#)), thus the intense build-up of O₂ we observe in our models may serve to protect water from photodissociation, lowering mass loss rates. Furthermore, the photochemical production of ozone (O₃) from free O₂ would be highly active on a planet with an over abundance of free oxygen ([Meadows et al., 2018b](#); [Segura et al., 2005](#)), increasing the amount of UV shielding molecules and greenhouse gases in the atmosphere. CO₂, prevalent on all the terrestrial planets with atmospheres in the Solar System and considered a likely constituent of any TRAPPIST-1 planetary atmospheres ([Krissansen-Totton & Fortney, 2022](#); [Lincowski et al., 2018, 2022](#); [Lustig-Yaeger et al., 2019a](#)), is also an important constituent to consider in super heated planetary atmospheres. CO₂ may prolong escape through heating, or bottleneck escape through cooling effects in the middle and upper atmosphere ([Kulikov et al., 2007](#); [Wordsworth & Pierrehumbert, 2013](#)).

Geological evolution, particularly a magma ocean phase, will be present and active during the hydrodynamic escape regime, with the attendant processes of water trapping in the mantle, outgassing, and the removal of oxygen or other species from the atmosphere ([Barth et al., 2021](#); [Krissansen-Totton & Fortney, 2022](#)). Hydrodynamic escape of a steam atmosphere is typically thought to be accompanied by a magma ocean phase ([Acuña et al., 2021](#); [Hamano et al., 2013](#)), as water provides a significant greenhouse effect that can prolong crustal solidification time. A magma ocean may also prolong periods of escape by slowing the supply rate of water to the atmosphere, effectively reducing cumulative water loss. However, though cumulative water loss would be reduced, the atmosphere itself may be dry for larger initial water contents when including a magma ocean due to water trapping in the mantle ([Barth et al., 2021](#)). A magma ocean would also suppress rapid build-up of atmospheric oxygen, prolonging energy-limited escape and increasing planetary oxygen retention by trapping it in the mantle. However, as initial water content increases, atmospheric oxygen build-up may still be inevitable, even with a magma ocean ([Barth et al., 2021](#)). With a defined vertical structure (e.g., 1D atmospheric model), surface-atmosphere exchange during a magma ocean phase can be modeled explicitly, which would inform upwards transport of

atmospheric constituents.

4.4.2 Initializing & Changing Surface Water Content

As initial water content represents our broadest initial parameter space, planetary formation and late water delivery research could narrow the range of plausible initial conditions used as input, providing tighter constraints on predicted outcomes for planets in the system, and also conserving computational expense, which could enable an increase in model complexity leading to more realistic treatment. Here we conservatively assume formation and water delivery is complete by 1 Myr. However, if a longer formation and water delivery time caused escape to begin later when the incident XUV was lower, then cumulative water loss would be reduced, and the ratio of oxygen retained to water lost would be increased. However, [Raymond et al. \(2022\)](#) show that the growth of the TRAPPIST-1 planets was likely complete within a few Myr with the bulk of their water reservoirs likely accreted during formation, as late water delivery greater than 5% of 1 Earth mass would disrupt the orbital resonance we observe today. In this case, the timeline of our simulations is consistent with these model results, suggesting the planets would have been subjected to the earliest, and most intense, period of hydrodynamic blow-off.

Regarding initial water content, previous work shows the TRAPPIST-1 planets may have formed with or possess up to ~ 10 wt% water ([Acuña et al., 2021](#); [Agol et al., 2021](#); [Raymond et al., 2022](#); [Schoonenberg et al., 2019](#)), which would provide ~ 430 TO on a $1 M_{\oplus}$ planet, roughly consistent with the largest initial water inventories we considered. However, based on the recent T1-b and c observations [Greene et al. \(2023\)](#); [Zieba et al. \(2023\)](#), our work would suggest the planets could not have formed with several hundreds of TO. The lower limit on initial water content, however, is relatively unconstrained by formation studies and extends to 0 for most planets ([Raymond et al., 2022](#)), which would remain plausible given the findings of this study, unless T1-c is later confirmed to possess atmospheric oxygen (see §4.3.2). Overall, our timeline of water loss and initial water contents considered are within a plausible range given recent formation and water delivery scenarios, but computational expense may be conserved by exploring a narrowed range of initial water contents.

5 Conclusions

We have shown the plausible range of water loss and abiotic oxygen production on the TRAPPIST-1 planets due to hydrodynamic thermal atmospheric escape using an updated VPlanet model ([Barnes et al., 2020](#)) and the most recently available constraints on the TRAPPIST-1 system ([Agol et al., 2021](#); [Birky et al., 2021](#)). We find the interior planets T1-b, c, and d, are likely desiccated for all but the largest initial water contents (>60 , 50, & 30 TO, respectively), and are at the greatest risk of complete atmospheric loss due to their proximity to the host star. However, they may still retain significant oxygen at very large initial water contents depending on assumed sink processes. The outer planets likely retain some fraction of water for all but the lowest initial water contents (~ 1 TO). We find T1-e, f, g, and h lose, at most, approximately 8.0, 4.8, 3.4, and 0.8 TO, respectively, corresponding to maximum oxygen production values of approximately 1290, 800, 560, and

90 bars, respectively. Additionally, we have found oxygen retention efficiency may vary widely across distance and initial water content, with rates $<10\%$ for close in planets with low initial water up to rates of $>80\%$ for distant planets, and those with high initial water.

Using currently available JWST observations for both T1-b and c (Greene et al., 2023; Zieba et al., 2023), our work constrains planetary initial water content, and suggests that the outer planets may still possess water at present-day. In the case of an airless T1-b, and a T1-c with a positive oxygen detection, an initial water content of $8.2^{+1.5}_{-1.0}$ would be most likely from our study, in agreement with predictions of Zieba et al. (2023). Assuming the outer planets are endowed with comparable initial water, an initial content of 8 TO implies T1-e, f, g, and h all likely possessed $\gtrsim 1.5$ TO after HZ entrance, with the predicted amount increasing with orbital distance. If T1-c is found to be airless, we suggest a basic upper limit on initial surface water of 9 TO and Zieba et al. (2023) suggest an initial water content upper limit of ~ 4 TO. Note, an initial water content of 4 TO does not definitively lead to desiccation on the outer planets in our work, which is in agreement with Krissansen-Totton (2023). These conclusions motivate follow-up observations to search for the presence of water vapor or oxygen on T1-c, and future observations of the outer planets in the TRAPPIST-1 system, which may possess substantial water.

Future model upgrades could include implementing a vertical atmospheric structure to enable more detailed escape rate calculations, additional atmospheric species, photochemistry, and surface sinks. As we move into a new era of observation, current work and future studies will assist in defining the plausible environments we could encounter, and statistical studies will be key to retrieving likely evolutionary histories.

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7 Chapter Appendix

7.1 Predicting Initial Water Content from a Final State

In Section 3.3.1 we showed the most likely initial water content our model would predict to reproduce a known present-day predicted or observed water content on the planet. Here, we

detail the generalized method used to achieve this result.

To start, let's assume we have constraints on a planet's present-day water content from either observation or simulation, and models that map initial water content to final water content. For each initial water content in our sampling grid, there are a sufficient amount of simulations (typically $\sim 3500 - 5500$ in our work) to encompass the uncertainty in the planet and host star's physical parameters, which in turn define the uncertainty in the final water content at a particular initial content. The question we then pose here is how to determine which initial water content on our sampling grid best produces the final state from our present-day constraints.

The first step is to model the planet's present-day water constraints with a probability density function (PDF) to assign probability weighting to final water contents based on the defined uncertainty in the constraints. In this work, we tested several common statistical functions and identified a gamma profile to best fit the present-day constraint we adopt. Gamma profiles worked well since the water mass fractions are restricted to be greater than or equal to 0 and, consequently, show asymmetric tails, but any continuous probability distribution may be used here in theory. With a gamma profile, our present-day water PDFs are described by:

$$f_i(w, a) = \frac{w^{a-1} e^{-w}}{\Gamma(a)}, \quad (3.2)$$

where i denotes which planet the PDF is describing (T1-b, c, d, e, f, g, or h), w is the present-day water content, a is the shape parameter, $f_i(w, a)$ is the relative likelihood of present-day water content w on planet i , and $\Gamma(a)$ is the gamma function evaluated at a particular shape parameter.

With the PDF describing the present-day water constraints, the next step is to determine the value of the PDF at the final water content predicted by each individual simulation across a particular initial water content. We then sum the PDF value across the individual simulations of a given initial water content and normalize for the total number of simulations in that suite to obtain a probability weighting for that particular initial water content. To normalize the probability weightings per initial water content, we divide by the number of simulations in the PDF value summation:

$$\text{Normalized Likelihood} = \frac{\sum_{z=1}^N f_i(w_z, a)}{N}, \text{ per initial water content,} \quad (3.3)$$

where $f_i(w_z, a)$ is the PDF for the planet being considered (Equation 3.2) evaluated at the final water content of a particular simulation, w_z , and N is the total number of simulations at that initial water content.

The initial water content with the highest probability weighting is the one that best produced the assumed present-day water constraints. If the initial water content grid is sampled finely enough, we can interpolate across our distribution of probability weightings to determine where the true most likely initial water content would be, and what the confidence intervals are on that prediction. This next step can only be taken if the grid of initial water contents with simulation data is fine enough that the distribution of probability weightings

appears to be a smooth, continuous curve; in some cases this may require running more data once the initial peak probability weighting has been identified. With sufficient data, this interpolation can be accomplished with a Riemann sum. To perform the Riemann sum, we take the curve of probability weightings versus initial water content and create area bins based on the data points, then find at what initial water content is the area under the curve 50% of the total area – the 50th percentile, or median value (i.e., the initial water content most likely to produce the present-day constraints). Then finding the bounds of 68% and 95% area under the curve, centered at the median value, will yield the 1σ and 2σ confidence intervals.

In our work, we created bins between adjacent data points with linear lines as the top of the bins. Thus, the area in a particular bin between two initial water contents, $IW1$ and $IW2$, is given by:

$$A_{bin} = \int_{IW1}^{IW2} (sx + b) dx = \left(\frac{s}{2}x^2 + bx \right) \Big|_{IW1}^{IW2} = \frac{s}{2}(IW2^2 - IW1^2) + b(IW2 - IW1) , \quad (3.4)$$

where s is the slope of the linear fit between the two data points and b is the y-intercept. This integrand is the same equation used to solve for a true value or confidence interval bound that lies between two data points. In fitting for the PDF this work, we used SciPy's stats module (Virtanen et al., 2020), and NumPy's polyfit routine (Harris et al., 2020b) for the linear fits.

CHAPTER 4

COUPLED PHOTOCHEMICAL-CLIMATE MODELING OF PLAUSIBLE TENUOUS OUTGASSED ATMOSPHERES ON THE TRAPPIST-1 PLANETS

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1 Summary

Available JWST observations TRAPPIST-1 system have suggested that several of the planets are likely airless, or possess a very tenuous atmosphere. However, the high atmospheric escape rates expected for these planets suggest that any tenuous atmosphere must be replenished by constant outgassing, and past studies on modeling potential atmospheres for the planets have not widely considered surface pressures $\ll 1$ bar. Here, we show that tenuous atmospheres on the TRAPPIST-1 planets are likely possible, supported by constant plausible rates of water and/or CO_2 outgassing against assumed high escape rates (up to $\sim 10^{30} \text{ s}^{-1}$). We use a coupled photochemical-climate model and sample from a broad phase space of outgassing, surface deposition, and top-of-atmosphere escape rates to test hundreds of atmospheres per planet. Critically, our model also allows surface pressure to vary based on the balance of sources and sinks. We find that 6 different compositional archetypes are generated via H_2O and/or CO_2 outgassing across our phase space, and atmospheres commonly fall between $10^{-4} - 1$ bar. We find that potentially habitable surface environments are possible for TRAPPIST-1d and e at pressures between 0.05 – 2 bar and 0.5 – 1 bar, respectively. Where possible, we compare our models to JWST observational data for TRAPPIST-1b, c, d, and e; all atmospheres found in this study for these planets match available transmission data to $< 3\sigma$. However, emission data are consistent with atmospheric outcomes constrained to thin O_2 -dominated compositions for TRAPPIST-1b ($\lesssim 0.01$ bars) and c ($\lesssim 0.2$ bars), which may or may not contain trace SO_2 .

2 Brief Introduction

In this chapter, we employ fully self-consistent coupled photochemical-climate modeling in grid sweeps of simulations across a broad parameter space of outgassing, surface deposition, and top-of-atmosphere escape rates for all 7 TRAPPIST-1 planets to show there are a range of tenuous atmospheres that are plausibly maintained at present day, consistent with current JWST data and constraints on planetary interior evolution from solar system data (Thomas et al., 2025). The modeling approach of this chapter is novel in that we achieve self-consistency in both photochemical-climate and outgassing-escape balance, i.e., we are not forcing constraints on the atmospheric pressure, composition, or temperature.

To model a range of secondary outgassed atmospheres on the TRAPPIST-1 planets, we are informed by geochemical models that predict CO_2 , H_2O and SO_2 as prominent gases released from terrestrial interiors, as a function of planetary composition and overlying atmospheric pressure (Gaillard et al., 2021). For our simulations, we use the water and CO_2 outgassing rate distributions of Thomas et al. (2025) as input, along with an array of atmospheric sinks. We further explore the effect of trace SO_2 by testing the injection of 100 ppm, 0.1%, or 1% SO_2 in the bottom layer of all stable atmospheric models. Through this work, we explore

types of atmospheres that are both observationally and theoretically plausible for the planets with available data (T-1b, c, d, and e).

In Section 3, we describe the results of our atmospheric models, including their photochemical-climate profiles (§3.1); atmospheric spectra (§3.2); derived data-model Pearson Correlation Coefficients (which quantify the correlation between atmospheric models and transmission data when available, §3.3); and calculated available Gibbs free energy (§3.4). From there, we discuss the characteristics and processes governing the behavior of our stable atmospheres (§4.1); model comparisons to current JWST data (§4.2); considerations for future observing campaigns (§4.3); pressure-temperature profiles and habitability (§4.4); the feasibility of derived atmospheric escape fluxes (§4.5); the potential for chemical disequilibria false positive biosignatures (§4.6); and the study limitations (§4.7). We conclude in §5.

3 Results

Here we present the results of our atmosphere simulations, focusing on stable results that represent plausible atmospheres, and we then simulate spectra from the stable atmospheres to compare to existing JWST observations of the TRAPPIST-1 planets.

3.1 Properties of the Stable Atmospheres

Our study tested grid sweeps across a broad parameter space of different boundary conditions, which led to several stable atmosphere types, and many non-viable combinations. Table 4.1 shows the number of atmospheres that were stable and converged (from each outgassing source, and with or without SO₂), as well as the total number of tested atmospheres, for all planets. The most common failure modes for unstable atmospheres were 1) atmospheric runaway (where outgassing significantly exceeded loss processes), 2) complete atmospheric loss ($<10^{-10}$ bars, escape processes dominated), or 3) unstable surface pressure or temperature (oscillating between two values without converging). In the failure state of atmospheric runaway, the final pressure would typically be between 10 – 500 bars, but the main indicator of this state is that pressure would increase by $\gtrsim 1$ bar on every model iteration, indicating that gases are building up. While we present a set of stable atmospheric solutions for these planets, since we did not use a statistical sampling method, we cannot quantify the overall likelihood of an atmosphere over an airless case, and we cannot conclude if one composition is statistically more likely over another. Furthermore, as shown by Table 4.1, T-1f in particular had a notably lower number of stable atmospheres than even the more outer planets in the system (T-1g and h). In the case of T-1f, a higher number of models failed to achieve ‘global convergence’ as there would be more oscillations in a given pass through the *VPL Climate* model. It may be that a more relaxed convergence method could be used in the future, allowing a higher number of atmospheres for T-1f, which we further elaborate on in the discussion.

Planet	Total Stable without SO ₂	H ₂ O Outgassed (without SO ₂)	H ₂ O-CO ₂ Outgassed (without SO ₂)	Total Tested (without SO ₂)	Total Stable with SO ₂	Total Tested with SO ₂
b	21	15	6	448	11	63
c	114	76	38	448	97	342
d	175	134	41	448	163	525
e	224	200	24	703	606	672
f	4	0	4	512	0	12
g	17	0	17	512	4	51
h	27	0	27	448	60	81

Table 4.1: Number of total atmospheres tested and stable atmospheres for each planet as a function of outgassing composition (H₂O or H₂O-CO₂), and with or without the addition of a fixed mixing ratio of SO₂ at the surface (either 100 ppm, 0.1%, or 1%). While many stable atmospheres were found for T-1c, d, and e, the more outer planets (T-1f, g, and h) produced unstable results for water outgassing only, but several stable results when CO₂ was included. T-1b produced a sample of stable atmospheres, though less than T-1c, d, and e because of its proximity to the host star leading to a more irradiated environment. Since SO₂ was tested in 3 ways for every stable atmosphere, the total number of tested SO₂-bearing atmospheres is just 3× the second column, but this is explicitly calculated in the last column of the table. Including SO₂ also led to a number of stable atmospheres for all planets except T-1f, with a preference for smaller SO₂ amounts (i.e., 100 ppm versus 1%) as this would lead to a smaller perturbation from an already stable state. T-1f likely did not produce stable SO₂-bearing atmospheres because of undersampling; there were only 4 atmospheres stable for T-1f originally, so only 12 configurations with SO₂ were tested.

Which Planets Displayed Stable Atmospheres per Archetype						
Planet	H ₂ O Dominated	O ₂ Dominated From H ₂ O Outgassing	Mixed H ₂ O-O ₂	Mixed CO ₂ -CO	O ₂ Dominated From Mixed H ₂ O-CO ₂ Outgassing	Mixed O ₂ -H ₂ O-CO ₂
b		X	X	X		X
c	X	X	X	X	X	X
d	X	X	X	X		X
e		X		X	X	X
f				X	X	
g				X	X	X
h				X		

Table 4.2: For each planet, an X is shown if at least 1 stable atmosphere was found for a given archetype.

3.1.1 Atmospheric Composition

Across all of the stable atmospheres generated by outgassing that were identified, we found a pattern of 6 different atmospheric archetypes, though not every planet was found to have stable models for all 6. Table 4.2 shows a visual representation of which archetypes were found to be stable for each planet, and we describe them here. The first 3 archetypes could occur in atmospheres generated through water outgassing alone: steam-dominated (>90% H₂O volume mixing ratio, VMR, at the surface); dry O₂-dominated sustained by H₂O outgassing (>90% O₂ VMR at the surface); and mixed H₂O-O₂. The other 3 atmosphere archetypes occur as a consequence of combined H₂O-CO₂ outgassing: mixed CO₂-CO, dry O₂-dominated sustained by H₂O-CO₂ outgassing (>90% O₂ VMR at the surface), and mixed O₂-H₂O-CO₂. Note, two separate archetypes are listed as O₂-dominated, but they have different trace gas compositions, as one is supported by H₂O outgassing alone, and the other by a mix of H₂O-CO₂ outgassing. Furthermore, the ‘dominant’ constituent in the mixed atmospheric types (H₂O-O₂, CO₂-CO, and O₂-H₂O-CO₂) may vary case-by-case. For the T-1b and T-1d simulations, stable solutions were found for all archetypes except for H₂O-CO₂ outgassed O₂-dominated. The T-1c simulations found stable solutions for all archetypes. The T-1e simulations provided stable solutions for everything except the H₂O-dominated and mixed H₂O-O₂ archetypes. None of the H₂O outgassed archetypes were stable in our simulations for T-1f, g, and h because the outgassed water would quickly freeze out due to the colder temperatures. However, all H₂O-CO₂ outgassed archetypes were stable for T-1g. H₂O-CO₂ outgassed archetypes with the exception of mixed O₂-H₂O-CO₂ were stable for T-1f. Finally, for T-1h, only mixed CO₂-CO atmospheres were found to be stable.

Figure 4.1 shows example cases of several key gas mixing ratio and temperature profiles as a function of atmospheric pressure for the atmospheric archetypes identified in this study. These plots show the diversity and range of outcomes from the coupled photochemical-climate model generated from the outgassing fluxes and modulated by the escape rates. For each of TRAPPIST-1c and e (representative of the interior and outer planets), we show one case per stable atmospheric archetype, in addition to the same atmosphere with an SO₂

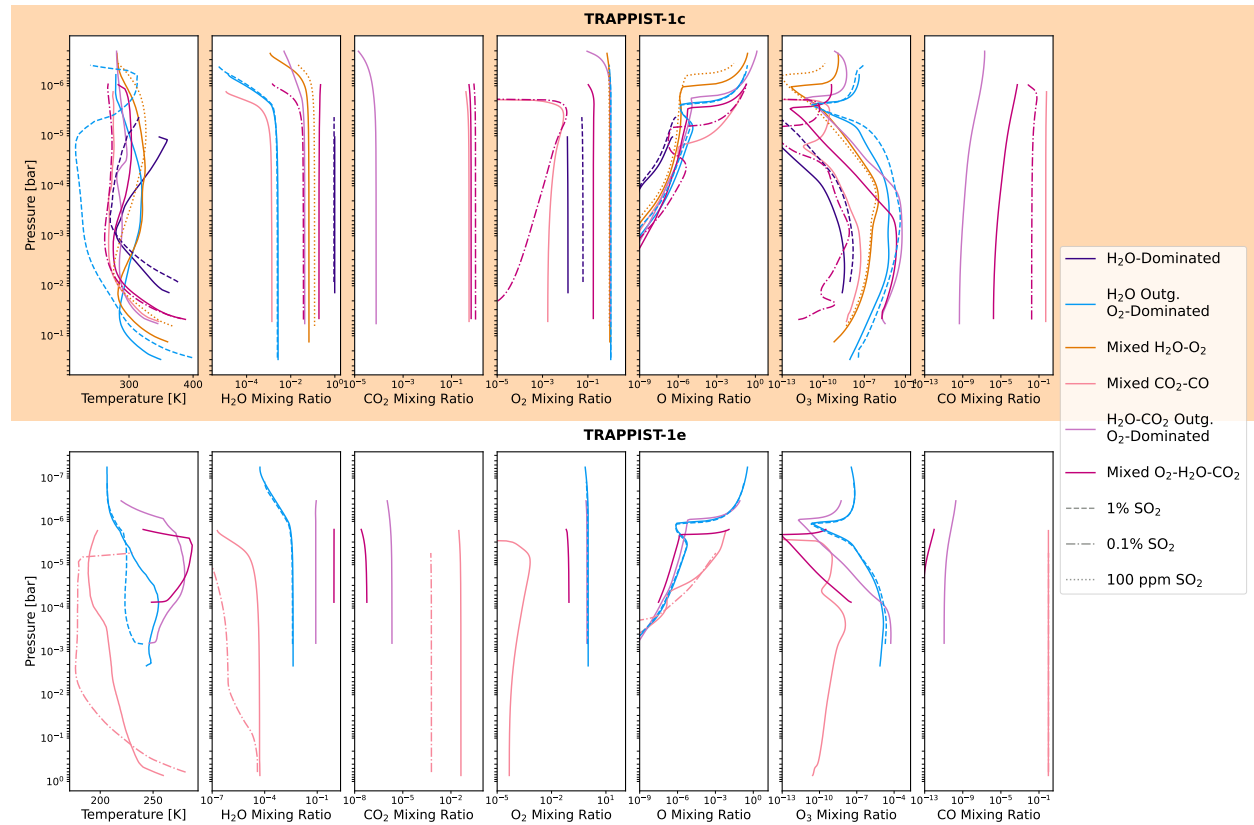


Figure 4.1: Examples illustrating the compositional and pressure-temperature range of the atmospheric archetypes found in this study. Temperature and gas mixing ratio profiles (as a function of atmospheric pressure) for H₂O, CO₂, O₂, O, O₃, and CO are shown for examples of every archetype atmosphere for T-1c and e. The top row (peach colored background) shows profiles for T-1c and the bottom row (white colored background) shows T-1e profiles. When available, atmospheric cases are shown both without (solid lines) and with SO₂ contributions of either 1% (dashed line), 0.1% (dashed dotted line), or 100 ppm (dotted line) injected into the bottom layer.

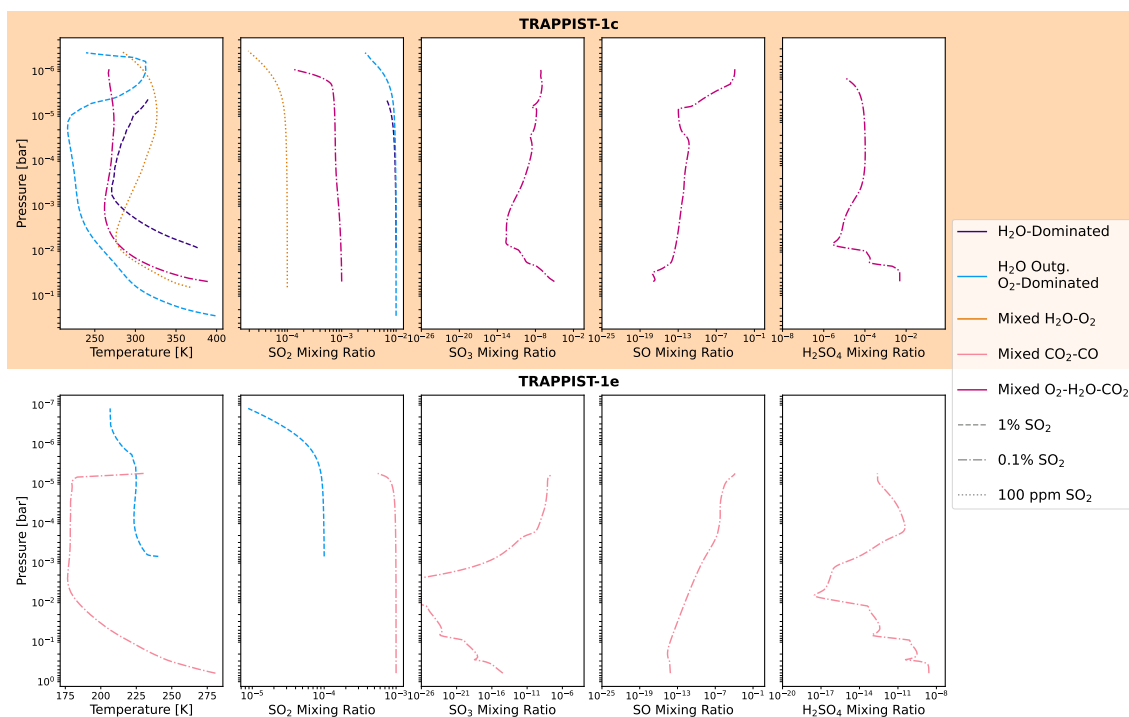


Figure 4.2: The volume mixing ratio profiles of SO_2 and daughter species for the same atmospheres given as examples in Figure 4.1 for T-1c and e. Format is the same as Figure 4.1.

addition, if available. The largest stable addition of SO_2 to a given atmosphere is preferred, i.e., if adding 1% SO_2 is unstable, but 0.1% is stable, then the 0.1% SO_2 result is shown. Additionally, for the SO_2 -bearing examples, relevant sulfur species are shown in Figure 4.2. The abundance of SO_3 , SO , and H_2SO_4 is negligible for all cases except the mixed O_2 - H_2O - CO_2 atmosphere for T-1c and the mixed CO_2 - CO atmosphere for T-1e.

The temperature profiles for almost all of the T-1c atmospheres display an adiabatic drop-off in the lower atmosphere, followed by a near isothermal profile. The exception is for the H_2O -bearing atmospheres, with the H_2O -dominated atmosphere providing the most pronounced example, which show heating in the upper atmosphere that is likely due to water vapor absorption. The T-1e temperature profiles are more varied, with the mixed CO_2 - CO atmosphere showing a similar behavior to the atmospheres of T-1c (drop-off and isothermal); the H_2O outgassed O_2 -dominated showing heating in the lower atmosphere, followed by cooling and more isothermal behavior in the upper atmosphere; and the H_2O - CO_2 outgassed O_2 -dominated and the mixed O_2 - H_2O - CO_2 atmospheres displaying heating in the lower atmosphere, followed by cooling in the mid to upper atmosphere. In general, the addition of SO_2 tends to lower the temperature of the atmosphere by reducing the water fraction.

As the only two possible outgassed species, the mixing ratio of H_2O and CO_2 , are mostly set by the source fluxes, particularly near the surface. The profiles of H_2O and CO_2 remain quite stable in every atmosphere, until the upper regions ($\sim 10^{-6}$ bar) where photolysis leads to a steady drop-off in H_2O , and to a lesser degree, CO_2 , and subsequent production of atomic

O, ozone, and slightly increased CO. The water profile for the T-1e SO₂-bearing mixed CO₂-CO atmosphere (pink dash-dot line, second row of panels, in Figure 4.1) significantly deviates from all other cases, showing a steep depletion of H₂O in the lower atmosphere, likely from reactions with SO₃. The O₂ profiles across all atmospheres remain quite stable and constant, until the upper atmosphere where photolytic destruction and TOA escape causes a drop in O₂ and production of atomic O. The loss of O₂ in the upper atmosphere is especially stark for the mixed CO₂-CO atmospheres for both planets and the SO₂-bearing mixed O₂-H₂O-CO₂ atmosphere for T-1c. The atomic O and ozone profiles are strongly tied to the photolysis of water and O₂, and subsequent recombination processes (particularly for O₃). Given surface deposition is in the lowest atmospheric layer and ozone destruction via reactions with OH also dominate in the lower atmosphere, ozone increases in abundance from the surface, hitting a peak in the middle atmosphere ($\sim 10^{-3}$ bars), and then decreasing towards the upper atmosphere. This slow decrease in ozone corresponds to an slow increase in atomic O, and both species show a sharp increase at the top of the atmosphere corresponding to the destruction of H₂O and O₂. Lastly, CO tends to increase very slowly as a function of altitude when it is a non-negligible constituent in an atmosphere, this is likely due to depositional loss at the surface and heightened production through CO₂ destruction in the mid and upper atmosphere.

3.1.2 Pressure-Temperature Phase Diagrams

Although potentially habitable surface temperatures are found for some of the atmospheric models we present, these atmospheres may also have extremely low pressures; in which case the physical conditions required to support liquid water on the surface of a planet may not be met, despite the promising temperature. To determine whether models with habitable pressure-temperature conditions exist, in Figure 4.3 we plot the pressure-temperature pairs for all of our simulations, superimposed on the phase diagram for water. The color of points corresponds to the atmospheric composition, and the shape (circle versus triangle) denotes the lack, or addition, of SO₂. Globally averaged (black borders) surface temperatures and pressures are shown for all planets, and day (yellow borders) and night (magenta borders) side values are additionally shown for T-1b, c, and d. The water phase diagram is split into a grey, blue, and red region indicating solid, liquid, and gas phases of water.

In terms of habitability, the globally averaged temperatures for T-1b and c are too hot and those for T-1f, g, and h are too cold, but several profiles of T-1d and e indicate potentially habitable pressure-temperature profiles. As expected, T-1b and c show very hot daysides and global averages, and very cold nightsides, many with hemispherically averaged temperatures below the freezing point of water. Some of the two interior planets' nightsides may even be temperate (between 273.15 – 300 K), though in all of these cases we use hemispheric averages. However, these averages lack the spatial resolution to accurately assess the potential for spatially-localized regions of extreme cold that could induce atmospheric collapse of the nightside. All atmospheres for T-1f, g, and h are within in the coldest region of the phase diagram, indicating water is likely in ice form, which is consistent with our result that none of these planets could sustain an atmosphere from water outgassing alone.

T-1d and e exhibit a range of stable atmospheres that produce above freezing surface temperatures in the global average. T-1 d is a very interesting case, existing right on the

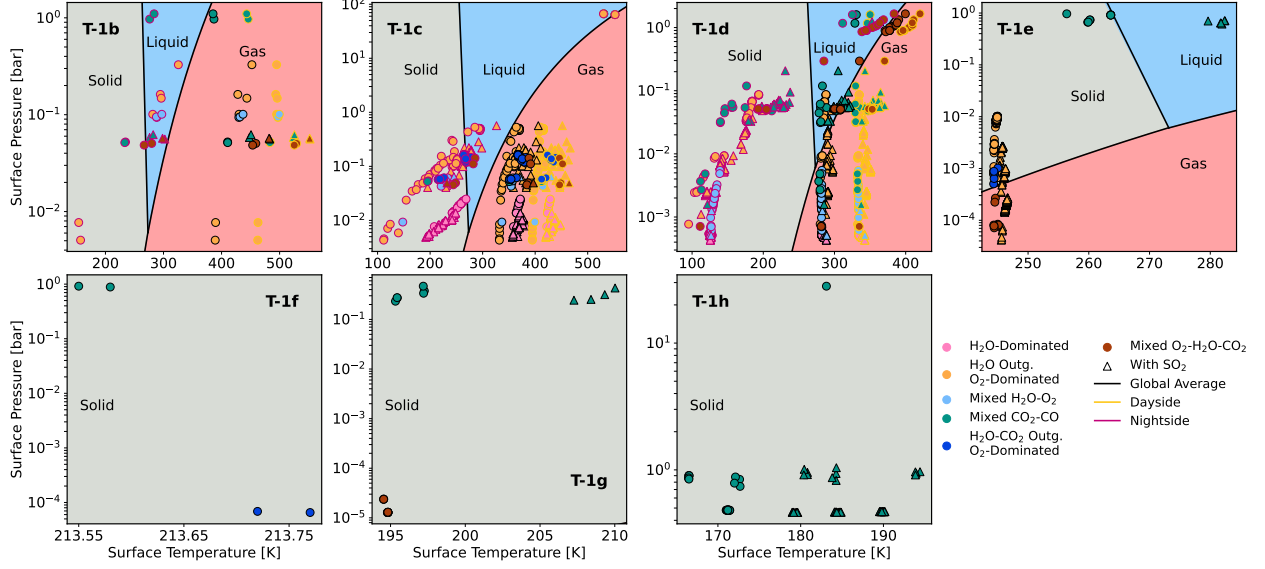


Figure 4.3: Surface pressure-temperature (P-T) points for each atmosphere in our work for each planet. Points are shown plotted over the phase diagram for water, where the grey, blue, and red shaded regions indicated solid, liquid, and gas phases. Points are colored by atmospheric composition (see figure legend). Globally averaged P-T pairs are shown with black borders, and dayside and nightside profiles for T-1b, c, and d are shown with yellow and magenta borders, respectively. Atmospheres containing SO_2 are shown by triangle points. T-1d and e both have atmospheres that may be fully contained in the liquid water region of the phase diagram.

inner edge of the potential habitable zone (e.g., Gillon et al., 2017; Meadows et al., 2023; Wolf, 2017); and notably, a few ~ 1 bar mixed CO_2 -CO atmospheres for T-1d have nightside, global average, and dayside temperatures all within the liquid water region of the phase diagram. In the case of T-1e, we found that only mixed CO_2 -CO atmospheres fall within the liquid water region, and that typically some addition of trace SO_2 was necessary to push the atmosphere solidly into this region.

3.1.3 Atmospheric Pressure & Escape Fluxes

Nearly all stable atmospheres found in this study have thin (< 1 bar) pressures and high O escape rates ($\sim 10^{26} - 10^{30} \text{ s}^{-1}$). As shown in Figure 4.3, the possible surface pressures for T-1b, c, and d range from 0.005 – 1 bars, 0.005 – 0.5 bars, and 0.0004 – 2 bars, respectively, with the exception of two high pressure outlier models for T-1c discussed below. For T-1e, f, and g, the surface pressures range from approximately $10^{-5} - 1$ bars, and for T-1h pressures range from 0.4 – 1 bars with the exception of one high pressure outlier simulation discussed below. However, we caution that the outer planets (T-1f through h), as well as T-1b, may be under-sampled, as stable atmospheres were difficult to maintain for the particular input combinations and convergence restrictions we tested (see Table 4.1).

There are a few surface pressure outliers for T-1c and h that likely possessed unrealistically low escape rates, allowing persistence of a massive atmosphere. For T-1c, there were two

stable high pressure (~ 60 bar) H_2O outgassed O_2 -dominated atmospheres which possessed O and O_2 escape rates approximately 1 order of magnitude less than many of the other, low pressure, O_2 -dominated atmospheres. Although O_2 does not exhibit strong spectral features at JWST-accessible wavelength ranges for atmospheres of 1 bar or less (Meadows et al., 2023), for higher pressure (> 3 bars) O_2 -dominated atmospheres, collisionally induced absorption from O_2 molecules can produce strong and broad features near 1.06 and 1.27 μm in transmission (Misra et al., 2014). Since these O_2 - O_2 features may be accessible to JWST for high enough pressures (Lustig-Yaeger et al., 2019a), and the outlying 60 bar T-1c atmospheres provide $\sim 3\sigma$ fits to the available data, these atmospheres are still included in further analyses. For T-1h, there is one outlying high pressure, ~ 30 bar, atmosphere which is nearly pure CO (produced by H_2O - CO_2 outgassing); this particular case was tested with negligible CO deposition and negligible CO_2 top-of-atmosphere (TOA) escape, so it was likely caused by an unrealistic build-up. However, since the CO deposition on exoplanets is extremely difficult to constrain, and because there is no public JWST data for T-1h, we decided to leave this unlikely high-pressure atmosphere in the remaining analyses of this study.

The maximum total escape flux of O, O_2 , and CO_2 across all atmospheres was $\sim 10^{30} \text{ s}^{-1}$. As previously described, we set TOA escape rates using an effusion velocity, as opposed to a strict fixed flux, to allow loss fluxes to respond to changing concentrations in the upper atmosphere; this is important because a fixed outgassing flux paired with fixed escape processes will not be able to dynamically evolve with the atmosphere (e.g., as composition or pressure changes). Here, we explore the resulting escape fluxes from our use of effusion velocities. Figure 4.4 shows the equilibrium escape fluxes found for every stable atmosphere; the top panel shows the O versus O_2 escape flux and the bottom panel shows O versus CO_2 . The dashed grey line on both panels indicates where the O and O_2 (top), or O and CO_2 (bottom), escape rates would be equal. Points with red rings highlight T-b and c modelled escape rates that produce atmospheres with spectra that are consistent with available emission data to within $< 1\sigma$ (Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023; Zieba et al., 2023). For comparison, we show the range of ion escape rates for TRAPPIST-1 planets assuming a Venus-like atmosphere, as constrained by Dong et al. (2018), as grey regions in Figure 4.4. In general, the O and O_2 escape rates of our best fitting T-1b and c models are high ($\sim 10^{27} - 10^{30} \text{ s}^{-1}$), and are equal to, or up to 3 orders of magnitude greater than the maximum escape rates reported by Dong et al. (2018) for a 1 bar Venus-like atmosphere. However, we note that neutral escape may be significantly larger (Brain & Hinton, *priv. comm.*) than the ion escape processes found by Dong et al. (2018) and these high escape rates in our study were balanced by the high end of plausible outgassing rates calculated in Thomas et al. (2025). While we did not statistically sample the outgassing rate distributions at high resolution, in general, stable atmospheres in this study required outgassing rates above the 50th percentile value of the distributions from Thomas et al. (2025). Finally, in regards to the escape rates presented in Figure 4.4, we would like to note that the ‘clumping’ sometimes seen for groups of simulations is likely an artifact of the sampling method (grid sweeps), not evidence that certain escape rates are ultimately preferred.

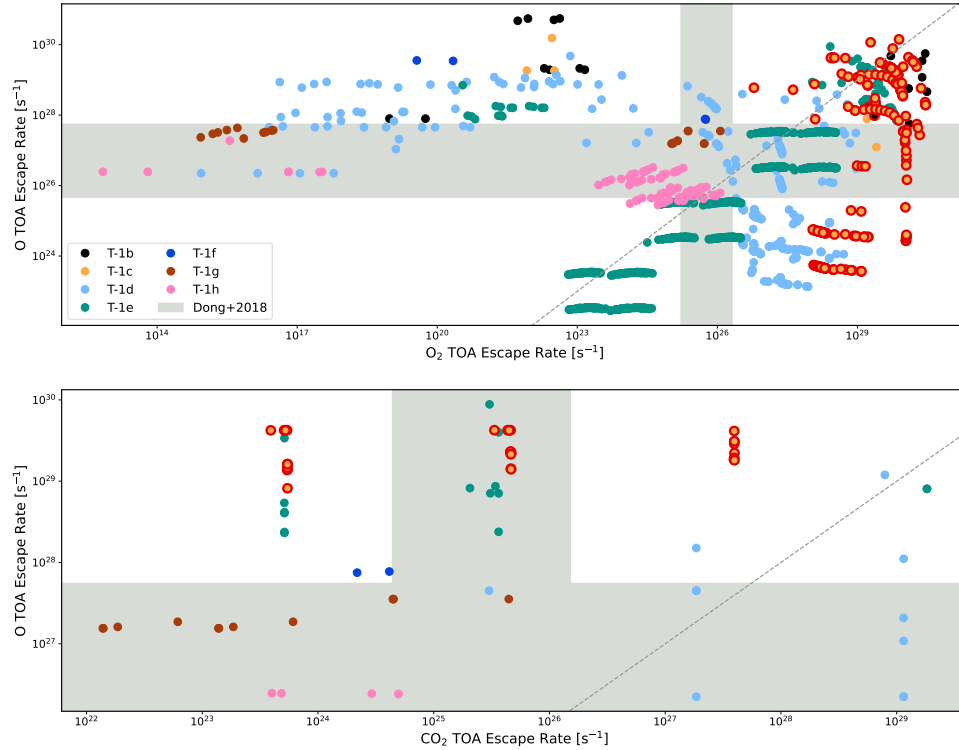


Figure 4.4: The escape fluxes (in s⁻¹) found across all stable atmospheres for all planets. Top panel shows the O versus O₂ escape flux, and the bottom panel shows the O versus CO₂ escape flux (for atmospheres including CO₂ outgassing). For T-1b and c, models that fit the available emission data to <3σ are denoted by red rings. The grey regions indicated the range of escape rates (across all 7 planets) found by [Dong et al. \(2018\)](#). The models that best fit the T-1b and c emission data tend to have higher O and O₂ escape rates.

3.2 Atmospheric Spectra and Comparison with JWST Observations

For each planet, we generated a summary figure that shows all the available model spectra, for comparison with known observational constraints from secondary eclipse, thermal phase curve and transmission spectroscopy measurements. In each figure, the spectra are colored by their fit to the available observational data, when applicable. We first discuss Figure 4.5 where we show the spectral results for T-1c, which has stable atmospheres for all compositional archetypes described above. In Figure 4.5, the top three rows (white background color) show the H₂O outgassed archetypes while the bottom three rows (grey background color) show the H₂O-CO₂ outgassed archetypes. The first column of panels shows transmission spectra in the wavelength range of 0.001 – 6.5 μ m, the second column of panels shows secondary eclipse (day-side emission) spectra in the wavelength range of 8 – 17 μ m, and the third column of panels (for the T-1b and c spectral plots only) show night-side emission averaged over the MIRI 15 μ m photometric bandpass, for comparison with available thermal phase curve measurements of the nightside emission (Gillon et al., 2026). The modeled transmission spectra are colored by their fit to the transmission data only (for T-1c, this is from Radica et al., 2025), while the emission spectra are colored by their joint fit to all available emission data, which can include secondary eclipse data and thermal phase curve data (for T-1c, Gillon et al., 2026; Zieba et al., 2023). Spectral features in Figure 4.5 (and subsequent spectra figures) are labeled by the absorbing gas.

The broad range of compositions for these atmospheres produce many characteristic spectral features, including for molecules that are chemically and photochemically generated from the outgassing products. As can be seen in Fig. 4.5, for the water-dominated outgassing atmospheres their spectra are, perhaps predictably, dominated by water vapor features in both the near- and mid-infrared. For the O₂-dominated atmosphere produced by photolysis of outgassed water, which has the lowest fraction of water vapor of the three water outgassing atmospheres, relatively weak features from photochemically-generated O₃ are also seen. In contrast the atmospheres generated from H₂O/CO₂ outgassing show more complex spectra, because of the addition of the CO₂ and its photochemical byproducts such as CO and O₃. For these atmospheres the spectra show weaker features from H₂O, when compared to the H₂O outgassing cases, additional features from CO and strong CO₂ absorption, as well as stronger features from O₃, including at mid-infrared wavelengths, when compared to those seen in the H₂O-only outgassing cases.

Considering the data-model comparison results for T-1c, the overall best-fit atmospheric archetypes for the available observations appear to be O₂-dominated regardless of outgassing source, and mixed H₂O-O₂ atmospheres (second, third, and fifth rows of Figure 4.5). Most atmospheres found here for T-1c are consistent with transmission data (Radica et al., 2025) to between 2 – 3 σ but, given the extreme difficulty in perfectly removing stellar contamination from transmission observations of TRAPPIST-1 (e.g. Lim et al., 2023; Rackham et al., 2018; Rathcke et al., 2025; Zhang et al., 2018), we conclude that there is not sufficient confidence to rule any of these atmospheres out. However, H₂O-dominated atmospheres (top row Figure 4.5) are slightly worse fits to the transmission data (at $\sim 3.1\sigma$) than all other archetypes. Looking at comparisons with the emission data for T-1c (Gillon et al., 2026; Zieba et al., 2023), which is more robust against stellar contamination, mixed CO₂-CO atmospheres

(fourth row, second column, Figure 4.5) provide the worst fits at $>3\sigma$, followed by mixed $\text{O}_2\text{-H}_2\text{O-CO}_2$ atmospheres (bottom row, second column Figure 4.5) at $2 - 3\sigma$. Both of these atmosphere types produce strong absorption at $15\mu\text{m}$ from CO_2 , and this is not seen in the data. Although they were least preferred in transmission, H_2O -dominated atmospheres (top row, Figure 4.5) fit T-1c emission data moderately well from $0.1 - 1.2\sigma$, with the lower pressure atmospheres providing a better fit. The best-fitting atmospheres overall for T-1c are O_2 -dominated atmospheres that had a surface pressure <0.2 bars (second and fifth rows, Figure 4.5), and the mixed $\text{H}_2\text{O-O}_2$ atmospheres (third row, Figure 4.5), which all fit the emission data to $<1\sigma$.

The spectra summary figure for T-1b is given by Figure 4.6, the layout is the same as Figure 4.5 except T-1b had no stable atmospheres for the H_2O -dominated and $\text{H}_2\text{O-CO}_2$ outgassed O_2 -dominated archetypes, so those rows are not included. All stable atmospheres identified for T-1b match the available transmission data (Lim et al., 2023) to $<1\sigma$. However, the data error bars are 60-100ppm, which is larger than the extent of many spectra features in this wavelength range, and large uncertainties in transmission may still be exacerbated by unremoved stellar contamination. In terms of emission data, almost every atmosphere archetype we modeled is ruled out to high ($>4\sigma$) confidence, except for two H_2O outgassed O_2 -dominated atmospheres with pressures of ~ 0.005 bars which fit the emission data at 2.3σ .

The spectra summary figure for T-1d is given by Figure 4.7, the layout is the same as Figure 4.5, except T-1d has no published emission data at the time of this study, so all spectra in both the transmission and emission plots are colored by their fit to the available transmission data (Piaulet-Ghorayeb et al., 2025); T-1d also had no stable $\text{H}_2\text{O-CO}_2$ outgassed O_2 -dominated atmospheres, so that row is absent from the figure. All atmospheres found for T-1d in this study fit the available transmission data (Piaulet-Ghorayeb et al., 2025) to $<1\sigma$, but as above, the extent of the data error bars exceeded the size of spectral features in all cases.

For T-1d, there was a very strong difference in the thermal features seen for atmospheres generated by the two different outgassing modes. While the water outgassing atmospheres produced largely featureless thermal spectra, those stable atmospheres generated from $\text{CO}_2\text{-H}_2\text{O}$ outgassing showed a broad range of features due to CO_2 absorption. Figure 4.7 shows that subsets of the mixed $\text{CO}_2\text{-CO}$ and mixed $\text{O}_2\text{-H}_2\text{O-CO}_2$ atmospheres have weaker absorption, and so noticeably higher emission near the $15\mu\text{m}$ band. For the mixed $\text{CO}_2\text{-CO}$ atmospheres, the strongest to weakest absorption features occurred when the surface mixing ratio of CO_2 ranged from $\gtrsim 1\%$ to $\lesssim 10$ ppm. For the mixed $\text{O}_2\text{-H}_2\text{O-CO}_2$ atmospheres, most of the stable results had high ($>90\%$) CO_2 mixing ratios, leading to more absorption and low thermal emission at $15\mu\text{m}$ (~ 50 ppm). However, cases with only $\sim 20\%$ CO_2 and larger O_2 and H_2O contributions, the CO_2 absorption was weaker, and emission at $15\mu\text{m}$ was much higher.

The modeled spectra for T-1e, f, g, and h are all shown on Figure 4.8. The left column of Figure 4.8 shows atmospheres for T-1e, the top two panels of the middle column show atmospheres for T-1f, the bottom panel of the middle column shows atmospheres for T-1h, and the right-most column shows atmospheres for T-1g. We do not include emission spectra for these outer planets (T-1e through h) as their cold temperatures mean emission photometry is less feasible. The layout is the similar to the left-most column of Figure 4.5, for T-1e this includes coloring by the model fit to the available JWST transmission data

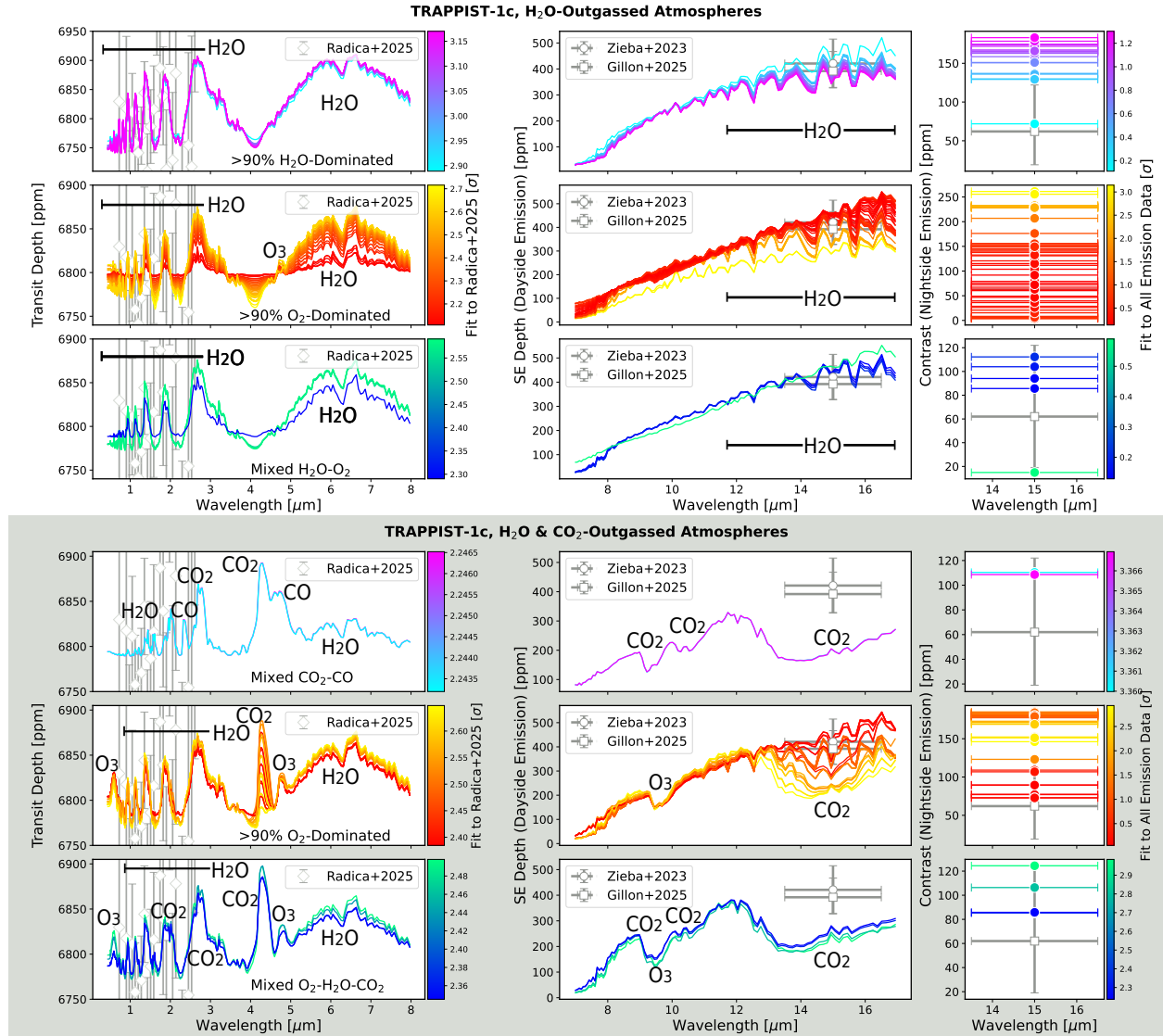


Figure 4.5: Transmission and emission spectra for all stable atmospheres found for T-1c (without trace SO_2). Top 3 rows (white background) and bottom 3 rows (grey background) show atmospheres sourced from H_2O and $\text{H}_2\text{O}-\text{CO}_2$ outgassing, respectively. Each row corresponds to a different atmospheric archetype (described in text), from top to bottom: H_2O -dominated, O_2 -dominated (produced via H_2O outgassing), mixed H_2O_2 , mixed CO_2 - CO , O_2 -dominated (produced via $\text{H}_2\text{O}-\text{CO}_2$ outgassing), and mixed O_2 - $\text{H}_2\text{O}-\text{CO}_2$. Left column shows visible to near-infrared transmission spectra ($0.001 - 6.5\mu\text{m}$), middle column shows secondary eclipse emission spectra at thermal wavelengths ($8 - 17\mu\text{m}$), and right column shows nightside thermal emission at $15\mu\text{m}$. Transmission spectra are colored by their fit (σ -deviation) to available T-1c transmission data (Radica et al., 2025), and emission data are colored by their combined fit to all available emission data ($15\mu\text{m}$ day and night points; Gillon et al., 2026; Zieba et al., 2023). Spectral features are labeled with the absorbing gas. The overall best fitting atmospheres for T-1c include lower pressure (<0.2 bar) O_2 -dominated atmospheres (regardless of outgassing source) and mixed O_2 - H_2O atmospheres.

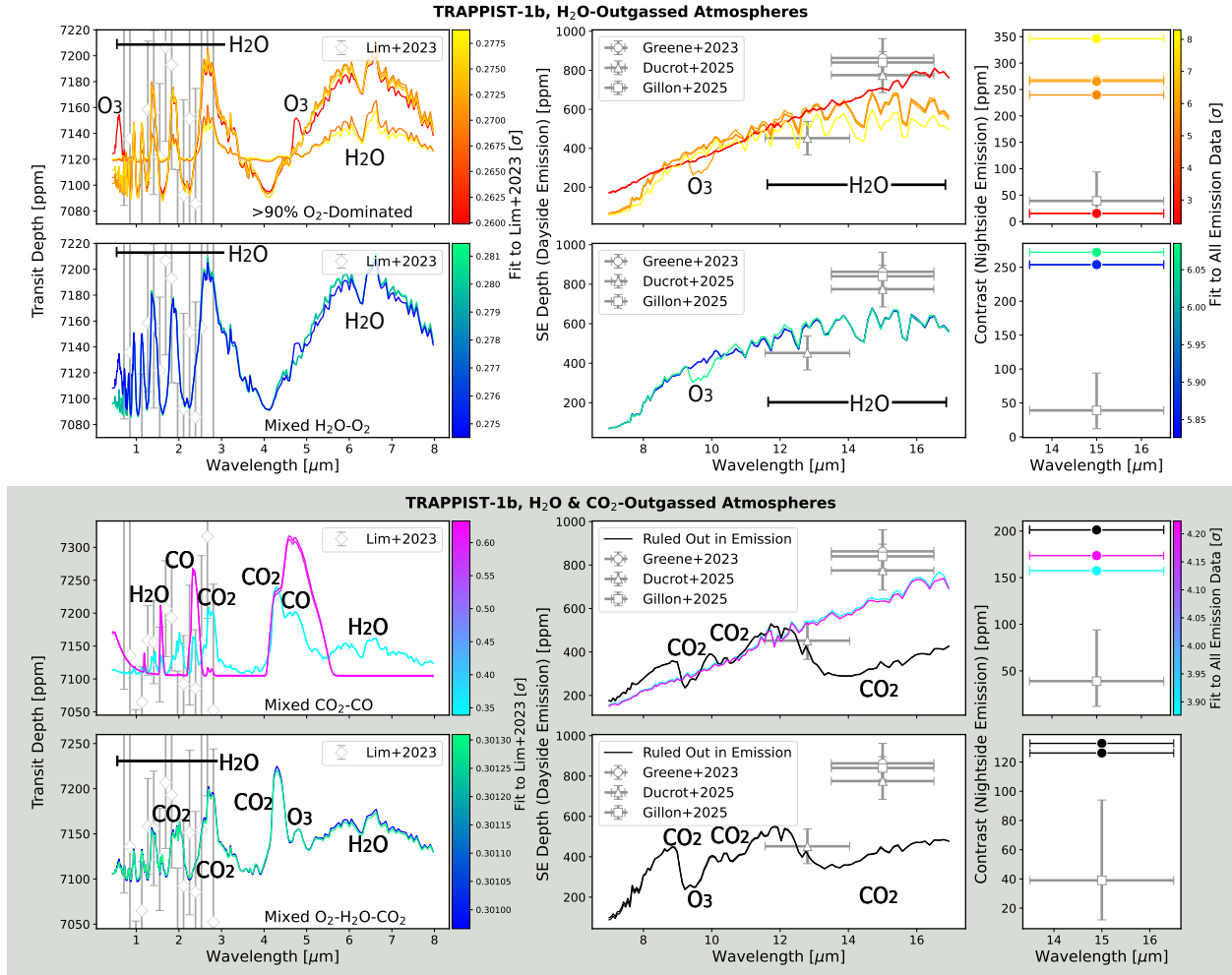


Figure 4.6: Transmission and emission spectra for stable atmospheres for T-1 b. transmission/emission columns and atmosphere archetypes (rows) are as for Figure 4.5, except that T-1b had no stable, realistic atmospheres of the H₂O-dominated or H₂O-CO₂ outgassed O₂-dominated archetypes, so those rows are not present. The only atmospheres that fit the T-1b emission data (Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023) to the $\sim 2\sigma$ level are H₂O outgassed O₂-dominated atmospheres with pressures of ~ 0.005 bars. The T-1b mixed CO₂-CO and mixed O₂-H₂O-CO₂ spectra shown in black indicate that they are confidently ruled out by emission data (fitting at a χ^2 of ~ 100).

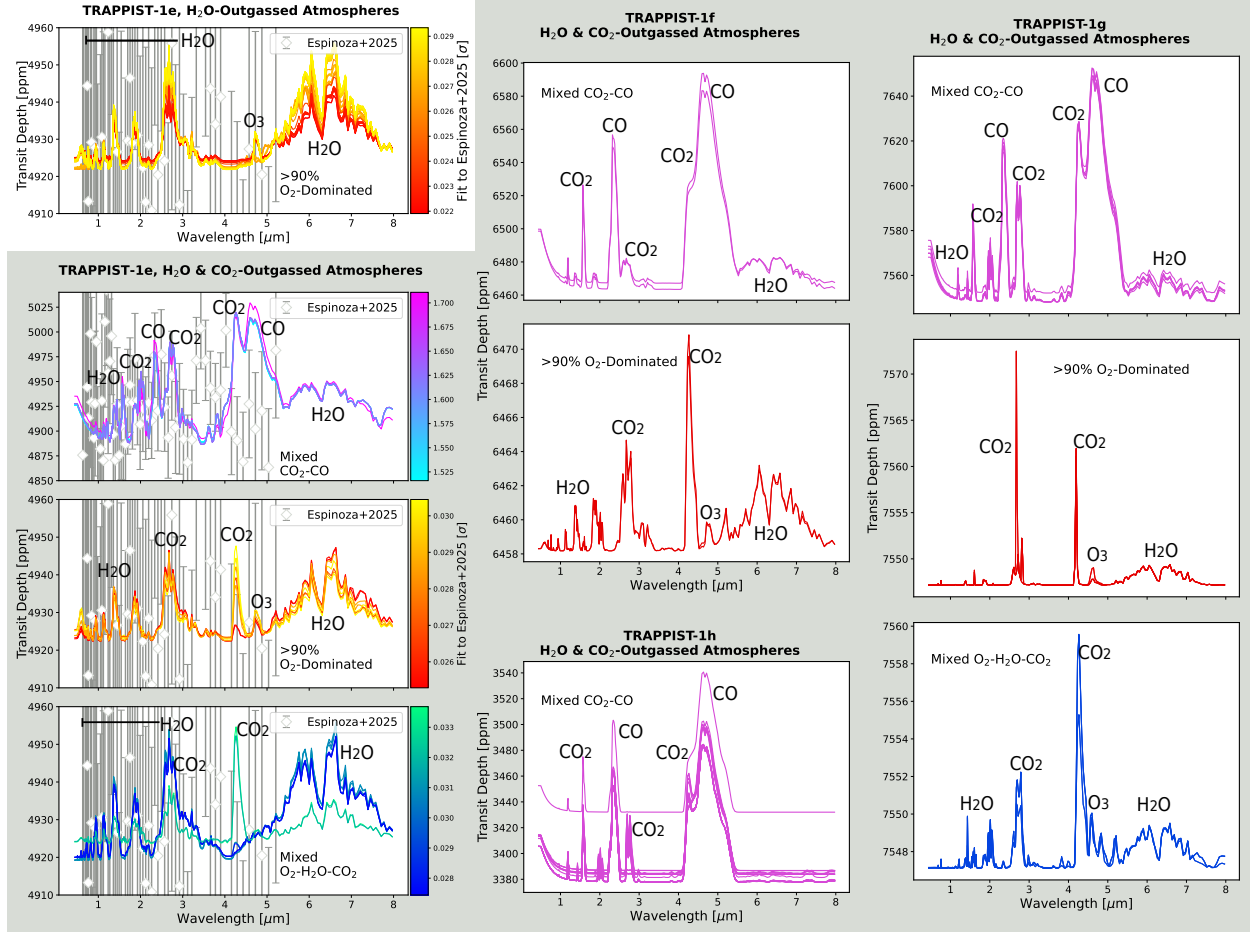


Figure 4.8: Similar to Figure 4.5, but contains the spectra for T-1e, f, g, and h. The left column shows transmission spectra for T-1e, and is laid out the same as the left column of Figure 4.5; spectra are colored by their fit to the recent T-1e transmission data (Espinoza et al., 2025; Glidden et al., 2025). T-1e has no stable H₂O-dominated or mixed H₂O-O₂ atmospheres. The middle column shows transmission spectra for T-1g, the top two panels of the right column show transmission spectra for T-1f, and the bottom panel of the right column shows transmission spectra for T-1h. T1-f, g, and h are too cold to sustain any stable atmospheres supported by H₂O outgassing alone. T-1g has all H₂O-CO₂ outgassed archetypes, but T-1f is missing mixed O₂-H₂O-CO₂ atmospheres and T-1h only has stable CO₂-CO atmospheres.

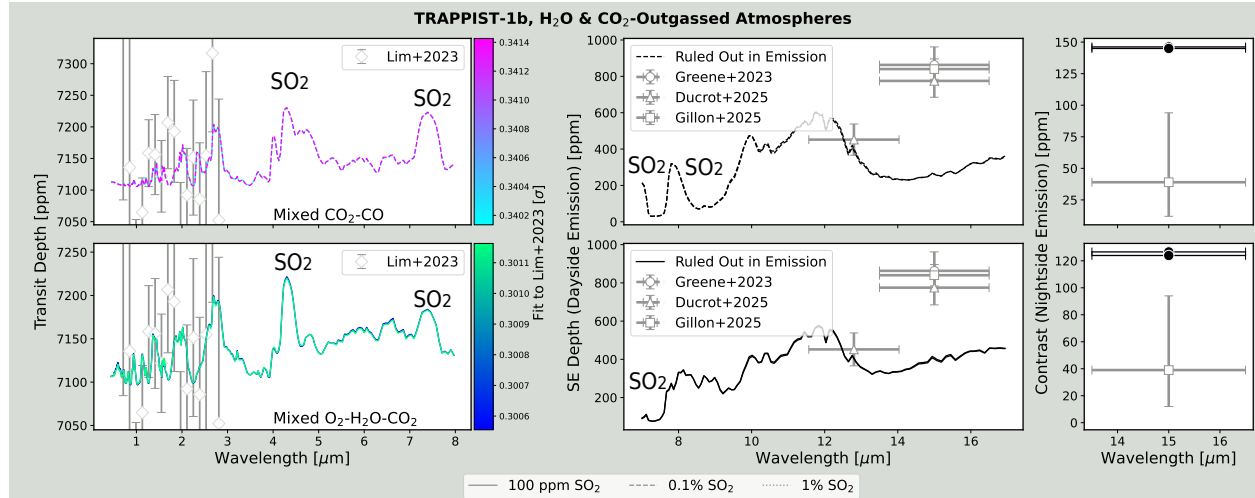


Figure 4.9: Same as Figure 4.5 but for the SO_2 -bearing atmospheres of T-1b. Solid, dashed, and dotted lines indicate that 100 ppm, 0.1%, or 1% SO_2 , respectively, was added to the bottom layer of the atmosphere. When including SO_2 , T-1b only had stable, realistic atmospheres for H_2O - CO_2 outgassed mixed CO_2 - CO and mixed O_2 - H_2O - CO_2 compositions. However, excessive heat redistribution rules out these compositions for T-1b based on the currently available emission data (Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023).

(Espinoza et al., 2025; Glidden et al., 2025). For T-1f, g, and h, which do not have available JWST data at the time of this paper, we plot spectra in one color, based on the atmospheric archetype shown.

Beginning with T-1e, no stable H_2O -dominated or mixed H_2O - O_2 atmospheres were found, but all other archetypes produced stable results. Furthermore, all modeled atmospheres fit the available transmission data (Espinoza et al., 2025; Glidden et al., 2025) to $<1\sigma$, except for the mixed CO_2 - CO compositions, which still fit the data to $<2\sigma$. For T-1f, g, and h, no atmospheres sustained by H_2O outgassing alone were found to be stable, as their lack of other greenhouse gases and corresponding cold temperatures lead to water condensation before substantial build-up or photolysis could occur. For T-1f, only stable mixed CO_2 - CO and H_2O - CO_2 outgassed O_2 -dominated atmospheres are found. For T-1g, all archetypes for H_2O - CO_2 outgassing are present; and for T-1h, only stable mixed CO_2 - CO atmospheres were found.

3.2.1 Spectra with Trace SO_2

For every stable atmosphere found in the H_2O only and H_2O - CO_2 outgassing suites, we tested 3 additional cases with the addition of fixed SO_2 mixing ratio of 100 ppm, 0.1%, and 1% at the bottom of the atmosphere; these SO_2 -bearing models were then rerun through our photochemical-climate modeling pipeline. Following the strategy of the previous section (§3.2), we provide a spectra summary figure that matches the layout of Figure 4.5 and shows all available SO_2 -bearing spectra for each planet. Notably, for planets with emission spectra, the addition of SO_2 creates a clear emission feature at $\sim 8.5\mu\text{m}$, increases emission seen just shortward of $15\mu\text{m}$, and dampens emission longwards.

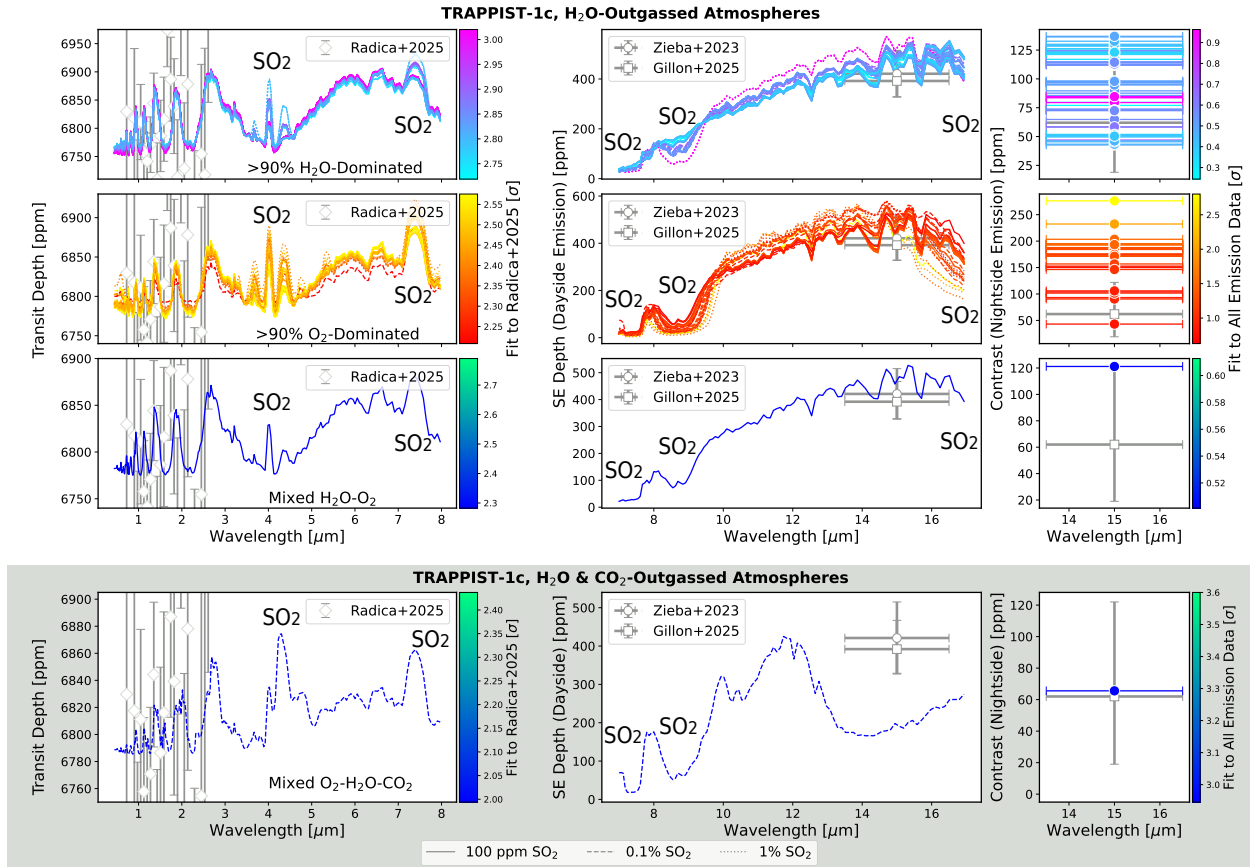


Figure 4.10: Same as Figure 4.5, but for the SO₂-bearing atmospheres of T-1c. Solid, dashed, and dotted lines indicate that 100 ppm, 0.1%, or 1% SO₂, respectively, was added to the bottom layer of the atmosphere. When including SO₂, no mixed CO₂-CO and H₂O-CO₂ outgassed O₂-dominated atmospheres were found to be stable, so those rows are not present in this figure. When including trace SO₂, all types of H₂O outgassed atmospheres may provide good ($<1\sigma$) fits to all available emission data.

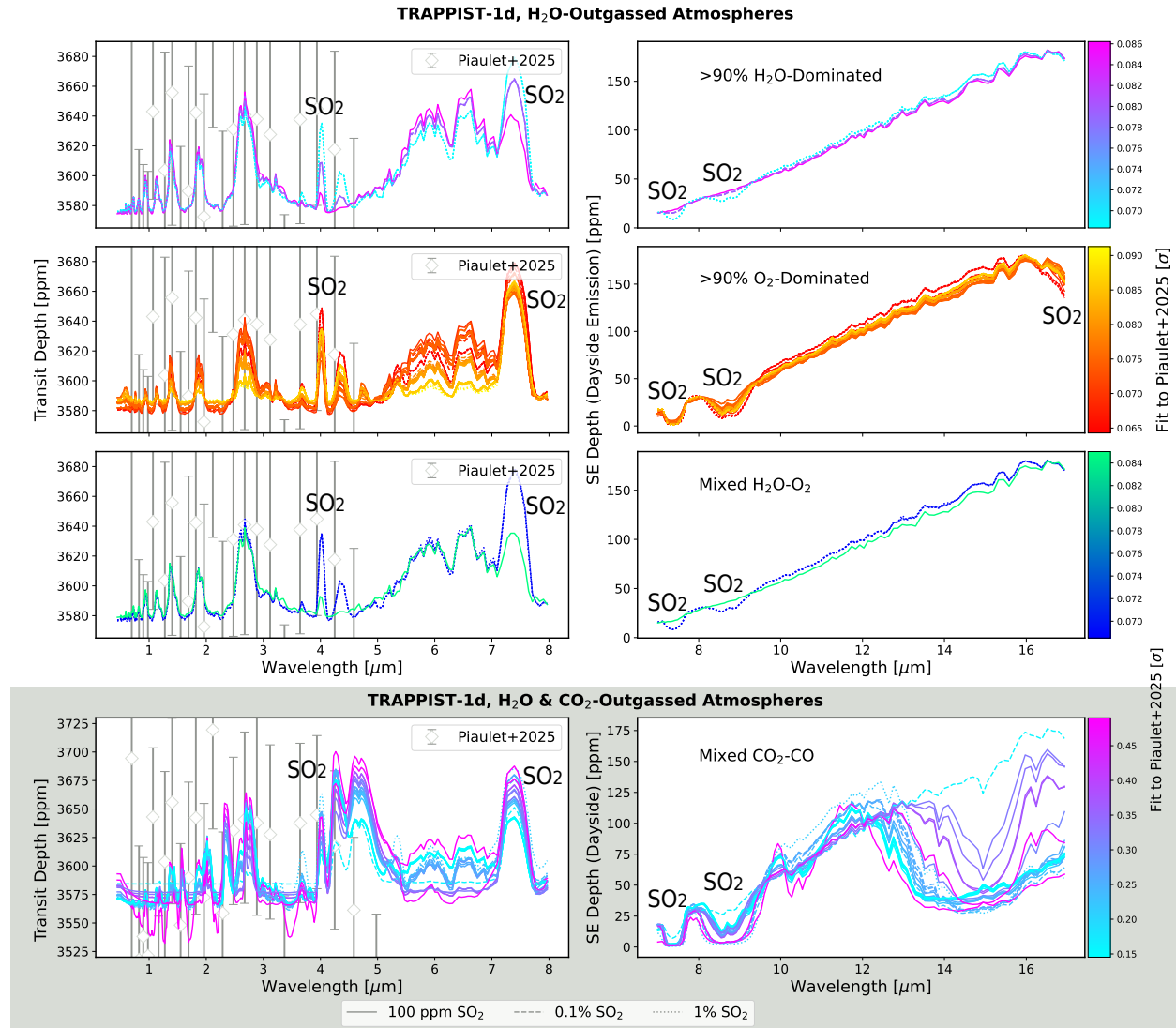


Figure 4.11: Same as Figure 4.5, but for the SO₂-bearing atmospheres of T-1d. Solid, dashed, and dotted lines indicate that 100 ppm, 0.1%, or 1% SO₂, respectively, was added to the bottom layer of the atmosphere. When including SO₂, H₂O-CO₂ outgassed O₂-dominated or mixed O₂-H₂O-CO₂ atmospheres were found to be stable, so those rows are not present in this figure. When including trace SO₂, the fit to available transmission data (Piaulet-Ghorayeb et al., 2025) is changed negligibly, with all atmospheres providing fits to $<1\sigma$.

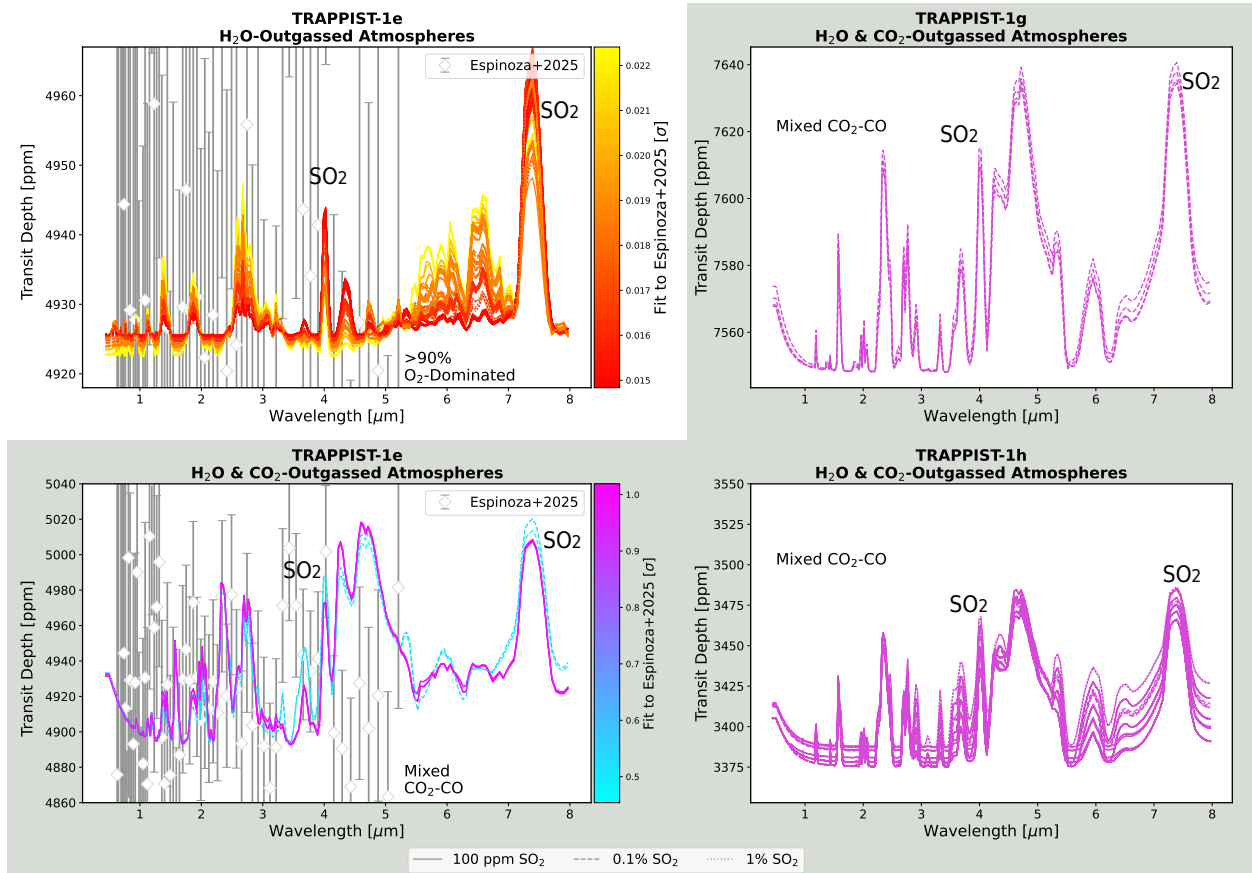


Figure 4.12: Similar to 4.5, but for the SO₂-bearing atmospheres of T-1e, g, and h. T-1f had no stable atmospheres containing SO₂ so it is not included here. The top and bottom left subplots show H₂O outgassed O₂-dominated and mixed CO₂-CO atmospheres for T-1e that contain trace SO₂; and the top and bottom right subplots show mixed CO₂-CO atmospheres with trace SO₂ for T-1g and h. Solid, dashed, and dotted lines indicate that 100 ppm, 0.1%, or 1% SO₂, respectively, was added to the bottom layer of the atmosphere.

Beginning with T-1b (Figure 4.9), the addition of trace SO_2 leads to stable, realistic atmospheres for only 2 compositions: mixed CO_2 -CO and H_2O - CO_2 outgassed O_2 -dominated. This is in contrast to the non- SO_2 results for T-1b, which also included O_2 -dominated and mixed H_2O - O_2 atmospheres. While the H_2O only outgassed O_2 -dominated and mixed H_2O - O_2 archetypes were stable without SO_2 , no stable examples were found when trace SO_2 was included. Similarly to the non- SO_2 -bearing cases, these spectra all match the T-1b transmission data (Lim et al., 2023) to $<1\sigma$. However, all stable SO_2 -bearing atmospheres for T-1b exhibited too much heat redistribution to match the available emission data.

When trace SO_2 was included for T-1c (Figure 4.10), all atmospheric archetypes produced by H_2O alone were found to be stable but, when CO_2 outgassing was included, only stable mixed O_2 - H_2O - CO_2 compositions were found, whereas the non- SO_2 results for T-1c also presented the other 2 possible CO_2 -bearing compositions. The addition of SO_2 moderately improved the fit of several H_2O -dominated atmospheres in emission (Gillon et al., 2026; Zieba et al., 2023), which all match to $<1\sigma$ in the SO_2 -bearing cases. The fits of other atmospheric archetypes to the emission data, as well as fits to transmission data (Radica et al., 2025) remain relatively unchanged with the addition of SO_2 .

For T-1d, when including trace SO_2 (Figure 4.11) all H_2O outgassed archetypes were stable, but only mixed CO_2 -CO compositions were found when mixed H_2O - CO_2 outgassed atmospheres were considered. Compared to the non- SO_2 cases for T-1d, only the mixed O_2 - H_2O - CO_2 archetype is missing when including SO_2 . The fits to available T-1d transmission data (Piaulet-Ghorayeb et al., 2025) for all atmospheres are improved when including SO_2 , however, they remain well below 1σ even before this SO_2 addition.

The SO_2 -bearing cases for T-1e, g, and h are shown on the same plot (Figure 4.12) to conserve page space; note, T-1f had no stable SO_2 -bearing atmospheres in our modeling suite, so it is absent from these results. When including trace SO_2 , mixed CO_2 -CO atmospheres were stable for all of T-1e, g, and h, and H_2O outgassed O_2 -dominated atmospheres were additionally stable for T-1e. Fits to the T-1e transmission data (Espinoza et al., 2025; Glidden et al., 2025) remained relatively unchanged by the addition of SO_2 (all $<1\sigma$). When including SO_2 , both T-1e and g are missing H_2O - CO_2 outgassed O_2 -dominated and mixed O_2 - H_2O - CO_2 atmospheres compared to the non- SO_2 cases.

3.3 Data-Model Correlation

To further analyze and assess our data/model comparisons, we calculated Pearson Correlation Coefficients (PCC; Section 3.0.1) for for all TRAPPIST-1 planets with observational data. The PCC correlation provides a means to assess if a given model predicts an increase or decrease in transmission depth at the same time that an increase or decrease is seen in a dataset. Specifically, absorption features in a spectrum are not independent, and a given molecule will provide a particular set of features in a spectrum. A positive PCC would indicate that a model predicts absorption at the same wavelengths that potential absorption is seen in the data.

The range of Pearson Correlation Coefficients (PCCs) are given by Figure 4.13, which shows the 1 and 2σ regions found from the distribution of PCCs across all stable atmospheres of a given archetype for a given planet. These results only pertain to the first 4 planets in the system (T-1b, c, d, and e) because the other planets do not have publicly available

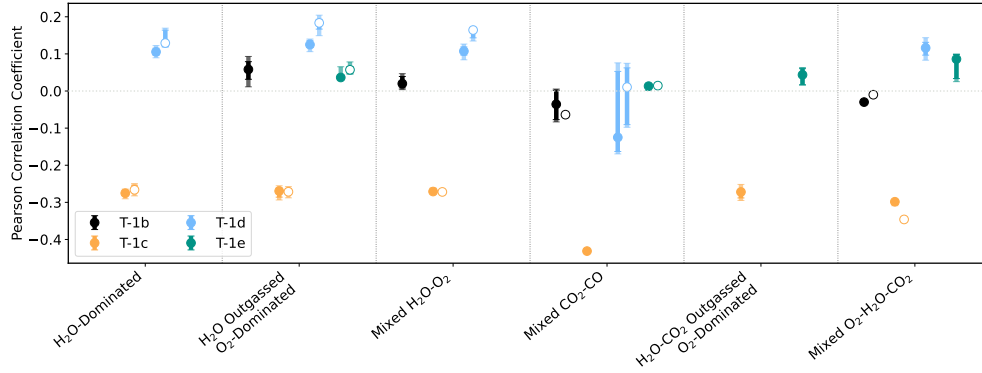


Figure 4.13: The 1 (darker colored bars) and 2σ (lighter colored bars) ranges of Pearson Correlation Coefficients (PCCs) when comparing all atmospheres of a given archetype for a given planet to the available JWST transmission data for that planet (T-1b, c, d and e). The bars with filled and unfilled circular points denote atmospheres without and with the addition of trace SO_2 , respectively. The dotted horizontal grey line shows where $\text{PCC}=0$, points that fall above that line indicate a positive correlation and points that fall below indicate a negative correlation to the transmission data.

transmission data to compare to at the time of this paper. In Figure 4.13, points with solid filled in circles correspond to the atmospheric archetype without the addition of trace SO_2 and points with unfilled circles include trace SO_2 .

Across our available models, correlation in either the positive or negative direction is generally weak ($< |0.10|$) for any atmosphere for planets T-1b, d, and e. Considering positive correlation as an indicator that the series of molecular features in the modeled transmission spectra may properly match the data, the atmospheric archetypes showing the strongest potential positive correlation to the T-1b data (Lim et al., 2023) are H_2O outgassed O_2 -dominated atmospheres. For T-1c, the PCCs suggest a moderately strong ($\geq |0.25|$) negative correlation between the transmission data (Radica et al., 2025) and all atmospheric archetypes found. Comparing to the T-1d data (Piaulet-Ghorayeb et al., 2025), all archetypes are generally positively correlated with equal strength ($\sim 0.1 - 0.15$), with the exception of mixed CO_2 -CO atmospheres which skew slightly towards stronger negative correlation. Lastly, considering the T-1e data (Espinoza et al., 2025; Glidden et al., 2025), all archetypes have negligible (~ 0.01) to weak (~ 0.1) positive correlation to the data, with the most positively correlated archetypes being H_2O outgassed O_2 -dominated and mixed O_2 - H_2O - CO_2 . The addition of SO_2 does not appear to significantly affect the PCC values for T-1b, c, and e, marginally raising the PCC for T-1e H_2O outgassed O_2 -dominated and T-1c mixed H_2O - O_2 atmospheres, but marginally lowering the PCC for T-1b mixed CO_2 -CO atmospheres, as well as T-1b and T-1c mixed O_2 - H_2O - CO_2 atmospheres. The addition of SO_2 does appear to raise the PCC values for all T-1d archetypes that produced stable SO_2 -bearing models.

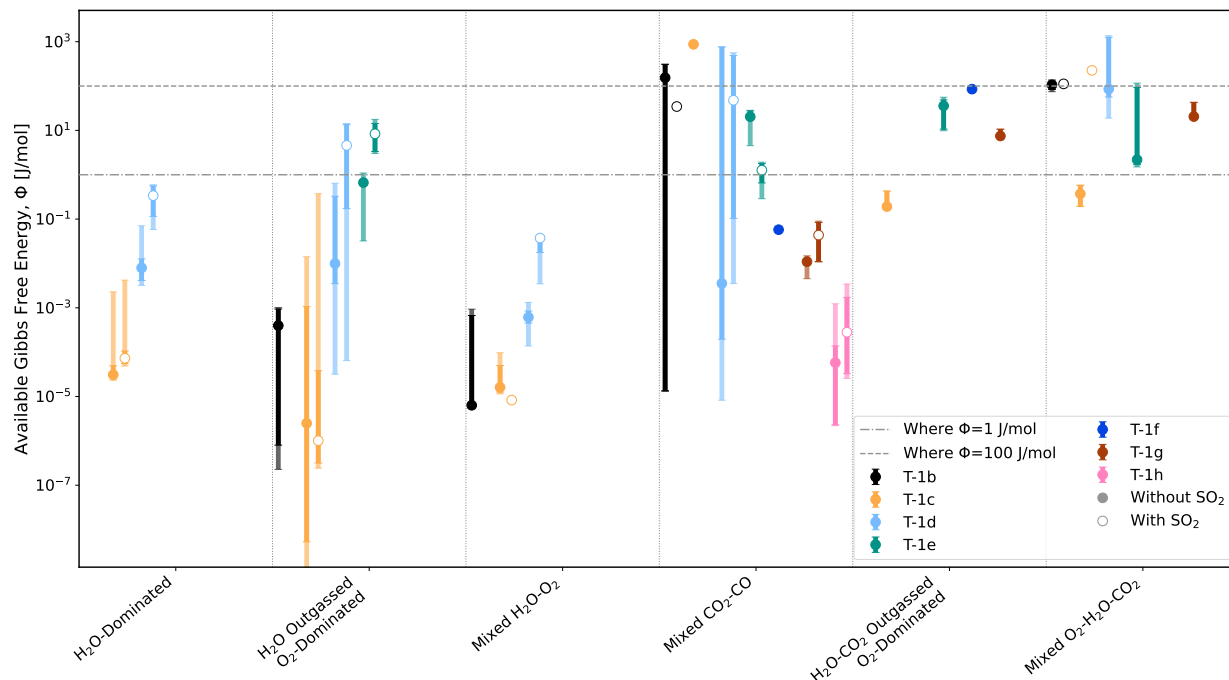


Figure 4.14: The 1 (darker colored bars) and 2σ (lighter colored bars) ranges of available Gibbs free energy for all atmospheres of a given archetype for a given planet. The bars with filled and unfilled circular points denote atmospheres without and with the addition of trace SO_2 , respectively. The atmospheres with the largest available Gibbs free energy (i.e., chemical disequilibrium) are those with a significant amount of CO and/or CO_2 .

3.4 Available Gibbs Free Energy

To assess the chemical disequilibrium state and potential for biosignature false positives of our outgassing sourced atmospheres, we follow the method of [Krissansen-Totton et al. \(2016\)](#) described in Section 4, and present the available Gibbs free energies of different atmospheric compositions for each planet in Figure 4.14. This figure shows the 1 and 2σ regions of the distribution of available Gibbs free energies found across all stable atmospheres of a given archetype for a given planet. Atmospheres produced through H_2O outgassing alone tend to have low (<1 J/mol) Gibbs free energy, but atmospheres with both H_2O and CO_2 source fluxes show a larger spread of available Gibbs free energy. The interior planets (b, c, and d) possess the atmospheres with the highest potentially available Gibbs free energy, in some cases >100 J/mol for mixed CO_2 -CO and mixed O_2 - H_2O - CO_2 archetypes. T-1c mixed CO_2 -CO and T-1d mixed O_2 - H_2O - CO_2 atmospheres may even produce an available Gibbs free energy exceeding 800 J/mol. The addition of SO_2 (unfilled circle points in Figure 4.14) either does not significantly affect the available Gibbs free energy or serves to increase it. In one of the most clearly differing cases, the addition of SO_2 in a mixed O_2 - H_2O - CO_2 atmosphere for T-1c served to increase the CO in the atmosphere through several reactions facilitated by S, HS, and HCO, which leads to a higher disequilibrium.

4 Discussion

Using a self-consistent photochemical-climate model that also accounts for the balance of plausible atmospheric outgassing and escape rates, we have demonstrated there is a broad range of stable tenuous atmospheres that could potentially exist on the TRAPPIST-1 planets. The stable atmospheres found in this study are constrained by reasonable rates of either H₂O or mixed H₂O-CO₂ outgassing (Thomas et al., 2025) and often exhibit thin (10 mbar – 0.1 bar) surface pressures, between that of Earth and Mars. Despite the overall model tendency toward low pressures, the compositions of these atmospheres vary widely, with a mix of compositions containing H₂O, O₂, CO₂, and CO. The expected high atmospheric escape rates driven by an M dwarf host star have raised concerns about the viability of thin atmospheres for planetary companions (e.g., Dong et al., 2018; Mansfield et al., 2024). However, we have shown that plausible replenishment from outgassing may allow tenuous secondary atmospheres to be maintained, even when adopting escape rates for O, O₂ and CO₂ (up to $\sim 10^{30}$ s⁻¹) that are many orders of magnitude higher than those seen for the Solar System terrestrials (e.g., up to $\sim 10^{25}$ s⁻¹ for neutral and/or ionized atomic O on Venus, Earth, and Mars; Gronoff et al., 2020).

We begin by discussing the properties of atmospheres in our modeling suite (§4.1) including photochemistry and spectral features. We then compare our models to current observational datasets of the system (§4.2) and consider how our atmospheric cases may be distinguished with future observations (§4.3). We further consider the implications for traditional planetary habitability that arise from our pressure-temperature profiles (§4.4), the feasibility of escape fluxes adopted by our models following our treatment of effusion velocities (§4.5), the identification of chemical disequilibrium false positive biosignatures (§4.6), and finally the limitations of our study (§4.7).

4.1 Characteristics of Atmospheres in this Study

Here we discuss the physical properties of the atmospheres modeled in this study. First we begin with a discussion of the photochemical profiles (§4.1.1), and then we describe the spectra seen across our atmospheres (§4.1.2).

4.1.1 Photochemical Profiles

The atmospheres in this study are sourced via outgassing, with vertical distributions and the generation of other gases governed by the destruction of outgassed H₂O, CO₂ and SO₂, and subsequent photolytic and inter-species reactions. For H₂O outgassing alone, the atmospheres found here are marked by efficient production of O₂, and to a lesser extent O and O₃, in the lower atmosphere. Post H₂O photolysis, the resulting O₂ can build up to a significant fraction of the atmospheric composition due to the loss of H to space. In the upper atmosphere, a sharp increase in atomic O and ozone is facilitated by high photolytic destruction of both H₂O and O₂. When including CO₂ outgassing, the general behavior of O, O₂, and O₃ remains similar, though production of these oxygen daughter species can also proceed via CO₂ photolysis. In some cases water vapor is at sufficiently low abundance that

CO₂ recombination is strongly inhibited (Gao et al., 2015), allowing CO (as well as O₂) to build up in the atmosphere, and even become the dominant constituent.

We find that the addition of SO₂ tends to reduce the amount of atmospheric O₂ and H₂O, particularly in the lower atmosphere, and increase the amount of CO. On examination of our photochemical reactions and products, we find that the availability of SO_x gases (e.g., SO, SO₂, SO₃) provides a set of catalytic reaction pathways that depletes O₂, often producing SO and O directly. Since SO₂ is more efficiently photolyzed in the upper atmosphere, the availability of S and SO leads to a steep drop-off of O₂ seen in some cases (such as T-1c’s O₂-H₂O-CO₂ profile in Figure 4.1). Water may be depleted with SO₂ more indirectly than O₂, with various reactions containing sulfur-bearing species using up OH, as well as a direct reaction with SO₃ to produce H₂SO₄ (e.g., Figure 4.2). CO tends to be increased in atmospheres containing SO₂ due to several production reactions involving S, SO, HS, and HCO.

We also found that the inclusion of SO₂ tends to increase ozone in atmospheres that do not contain CO₂ outgassing, and decrease it in those that do, compared to their baseline cases. For a water outgassed atmosphere, devoid of CO₂ and CO, the addition of SO₂ leads to increased destruction of OH via reactions with SO_x gases, thus ozone increases — as its primary destruction pathway with OH is suppressed. However, when CO₂ is also outgassed, OH is already suppressed by reactions with CO and consequently when SO₂ is added, it does not significantly change the availability of OH. Instead, SO_x gases can deplete O₂, reducing the source of ozone, and it can even destroy ozone directly. This leads to an overall reduction of ozone in a joint H₂O and CO₂ outgassed atmosphere when SO₂ is injected.

Considering inter-planetary comparisons, there are several notable results which appear to be a function of distance from the host star—including the stability of H₂O-generated atmospheres, and the strength of top-of-atmosphere escape. When considering all stable atmospheres per planet and comparing similar archetypes, the fraction of water vapor at the surface level of the atmosphere strictly decreases as distance from the host star increases. This is due to the colder atmospheric temperatures overall on the outer planets, and increased condensation and precipitation of water out of the vapor stage as the temperature drops. The escape rate of O₂ also tends to be higher for interior planets due to the increased incident radiation available to drive escape (e.g., Figure 4.4). There is a similar, but weaker, distance dependence for the escape rates of atomic O and CO₂; it likely appears weaker because of the smaller mass of atomic O (easier to remove), and due to undersampling in the case of CO₂ (i.e., there were a relatively small number of stable cases that contained CO₂ to consider).

In contrast to the globally-averaged pressure-temperature profiles for Solar System terrestrials, that exhibit cooling with altitude from the surface and an upper atmosphere with an isothermal profile or temperature inversion, several of our low surface pressure atmospheres displayed some unusual behavior. For TRAPPIST-1 e in particular, several model atmospheres show heating with altitude in the lower atmosphere, followed by cooling with altitude in the upper atmosphere. This behavior is most prominently seen for O₂-dominated atmospheres generated by the H₂O-CO₂ outgassing, and for mixed O₂-H₂O-CO₂ atmospheres (Figure 4.1). This behavior is driven by high atmospheric H₂O abundances in low surface pressure atmospheres ($\lesssim 10^{-3}$ bars), which allows more rapid heating in the lower atmosphere facilitated by absorption from the H₂O (see bottom row Figure 4.1).

4.1.2 Atmospheric Spectra

Turning to spectral features, the three H₂O outgassed atmospheric archetypes in this work (prior to the addition of SO₂) all show spectra dominated by H₂O features, as this is the most active absorber in these atmospheres. Atmospheres more strongly dominated by O₂ have lower water vapor abundance and display smaller water vapor features in transmission. This is similar in emission, where the spectral continuum is dampened by water vapor absorption from 12 – 17 μm . All of the H₂O outgassed atmospheres provide adequate fits to transmission data for all planets ($\lesssim 3\sigma$), as well as T-1c emission data, and the O₂-dominated atmospheres may provide $<3\sigma$ fits to the T-1b emission data. For a given atmospheric pressure, adding H₂O tends to increase nightside temperature and worsen the fit to the emission data (Gillon et al., 2026). Similarly, even for O₂-dominated atmospheres, higher pressures also increases the nightside temperature and result in poorer fits (e.g., $>2\sigma$ for >0.4 bars on T-1c). Ozone features are relatively absent from the H₂O outgassed atmospheres, likely because reactions with OH (derived from H₂O photolysis) destroy O₃, and prevent it from building up to significant levels in the atmosphere. However, weak O₃ features are seen in the O₂-dominated atmospheres where atmospheric water vapor is lower, and O₃ can persist and build up to higher abundances.

The joint H₂O and CO₂ atmospheres have more diverse compositions and a larger collection of spectral features, including features from CO₂, H₂O, CO, and O₃. In all of the compositions containing CO₂-outgassing, the strong absorption features of CO₂ (e.g. near 2, 2.7, 4.2, 9.4, 10.5 and 15 μm) can be seen with varying degrees of strength. Several smaller CO₂ features shortward of 1.5 μm can also be seen, though they may be hard to disentangle from H₂O features in the same region. CO is primarily seen in the spectra of the mixed CO₂-CO composition atmosphere spectra at 2.35 μm and 4.6 μm . There is also a 4.7 μm feature seen in the spectra of the H₂O-CO₂ outgassed O₂-dominated and mixed O₂-H₂O atmospheres. However, in these compositions it is caused by O₃ absorption as opposed to CO. The ozone Chappuis band additionally provides a relatively large feature spanning 0.5–0.7 μm , though this is difficult to access with JWST, especially for planets orbiting M dwarfs, which produce relatively little radiation for transmission at these shorter wavelengths.

When including SO₂ in the simulations, clear features appear primarily near 4 μm , 7.3 μm , and 8.5 μm , and the general continuum in emission is increased between ~ 10 – 16 μm and depressed at wavelengths longer than ~ 16 μm due to a broad SO₂ feature from 16 – 22 μm . In transmission, the clearest effect of including SO₂ is the presence of 3 absorption features centered about 4 μm , these are particularly well delineated in the H₂O outgassed O₂-dominated atmospheres (e.g., T-1c Figure 4.10, T-1e Figure 4.12). In emission, there is a large feature centered at ~ 8.5 μm , which becomes saturated particularly in O₂-dominated atmospheres (see T-1c, Figure 4.10). Furthermore, the overall emission continuum is raised (visible between ~ 10 μm to 16 μm) compared to the non-SO₂ atmospheres. When CO₂ is present, the SO₂ absorption at ~ 16 μm is not discernible from CO₂. Addition of greenhouse gas SO₂ and subsequent photochemical reactions tends to increase both the day and nightside temperatures of planets, raising the continuum. This effect can result in warming of up to 40 K on the dayside and 20 K on the nightside in the case of O₂-dominated atmospheres that have lower water abundances (Figure 4.3). In steam atmospheres, whose compositions are already dominated by a strong greenhouse gas, the addition of SO₂ does not significantly change the

temperature.

4.2 Model Comparisons to Current Data

When possible, we quantify the fit of atmospheres in this study to available JWST secondary eclipse, thermal phase curve and transmission data (using the χ^2 goodness-of-fit test) and show that most current observations are not sufficient to distinguish, or rule out, the thin atmospheres we modeled to $>3\sigma$. Transmission data is currently available for T-1b (Lim et al., 2023), c (Radica et al., 2025), d (Piaulet-Ghorayeb et al., 2025), and e (Allen et al., 2025; Espinoza et al., 2025; Glidden et al., 2025), and emission data is available for T-1b (12.8 and 15 μm ; Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023) and T-1c (15 μm ; Gillon et al., 2026; Zieba et al., 2023). The transmission data for TRAPPIST-1 planets is now known to be thoroughly affected by stellar contamination (Howard et al., 2023; Lim et al., 2023; Rackham et al., 2018; Rathcke et al., 2025), which, in combination with small datasets, has led to large error bars on transmission points ($\pm >100$ ppm) that exceed the size of even the largest spectral features for atmospheres in our study ($\lesssim 150$ ppm). Due to this uncertainty versus feature strength size difference, transmission data is currently not sensitive to the tenuous atmospheres studied here. The lack of sensitivity at the $>3\sigma$ to the tenuous (<0.1 bar) atmospheres in this work is in agreement with the conclusions reached by the studies presenting JWST transmission data (Espinoza et al., 2025; Glidden et al., 2025; Lim et al., 2023; Radica et al., 2025).

In emission, we find that only extremely thin ($\lesssim 0.01$ bar) dry O_2 atmospheres match the available T-1b data (Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023) to $<3\sigma$, which is in agreement with past work suggesting a lack of significant greenhouse gases or thick atmosphere (e.g., Ih et al., 2023). Conversely, several compositions match T-1c emission data (Gillon et al., 2026; Zieba et al., 2023) to $<1\sigma$ including O_2 -dominated atmospheres with no significant CO_2 at ≤ 0.3 bars or with $<1\%$ CO_2 up to 0.05 bars, O_2 -dominated with up to 15% H_2O at ≤ 0.06 bars, or H_2O -dominated at ≤ 0.02 bars. Additionally, nearly every atmospheric scenario for T-1c presented here are consistent at $\leq 3\sigma$ to the T-1c emission data (Gillon et al., 2026; Zieba et al., 2023). This is in agreement with past work on analyzing these observations (e.g., Lincowski et al., 2023) which found trace amounts of greenhouse gases (e.g., H_2O , CO_2) may be present in thin atmospheres or in atmospheres dominated by a less active constituent, such as O_2 .

After the comparisons with T-1e data given in Espinoza et al. (2025); Glidden et al. (2025), additional preliminary results of a multi-cycle JWST program by Allen et al. (2025) were published. However, these additional three T-1e transmission observations possessed comparable signal to data already available (Espinoza et al., 2025; Glidden et al., 2025) and did not change the confidence on distinguishing their best-fit atmospheric scenario from a flat line. Because the newly available data would not have changed the detection fits found in our results, we did not recalculate the χ^2 goodness-of-fit metric for our models. Future data from the multi-cycle program for T-1e may change the detection fits of models in this work when signal is increased. Notably, Allen et al. (2025) highlighted spectral features that may be attributed to CO , which will be tested with future observations in the multi-cycle program. While it is unclear if the potential CO absorption seen by Allen et al. (2025) would be more likely caused by the planetary atmosphere or stellar photosphere, our model

simulations did generate several atmospheres rich in CO, which may be sustained both with and without trace SO₂ (Figures 4.8 and 4.12). These high CO atmospheres for T-1e are all between $0.5 - 2\sigma$ fits to the T-1e transmission data from Espinoza et al. (2025); Glidden et al. (2025).

4.3 Distinguishing Atmospheric Scenarios & Future Observing

Even though many of the atmospheric spectra shown in Figures 4.5 through 4.12 are from 0.1 bar or even lower pressure atmospheres, they can still generate potentially observable 50-120 ppm features in transmission and emission spectra. The interior planets (T-1b, c, and d) in particular are hot enough that emission observations, which avoid the stellar contamination seen in transmission studies, can be used to learn about their atmospheres. However, JWST data for T-1b and c are primarily in the 15 μ m bandpass (Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023; Zieba et al., 2023), which is strongly sensitive to absorption from CO₂, but less compositionally diagnostic for atmospheres that don't contain it, which includes several of our O₂- and H₂O-dominated compositions. A drop in secondary eclipse depth, indicating a cooler dayside, can be due either to heat transport from the day to nightside by an atmosphere, or to CO₂ absorption, or a combination of both. To break this degeneracy for atmospheres that don't contain CO₂, absorption from additional diagnostic molecules, such as H₂O and O₃, needs to be sought.

For O₂-dominated atmospheres produced by either H₂O or mixed H₂O-CO₂ outgassing, the and T-1b and T-1c results (Figure 4.5, 4.6, 4.9 and 4.10) show that, beyond CO₂, the largest emission features are created when either trace O₃ or SO₂ is present at sufficient levels to create features at 10 and 8.5 μ m, respectively. In the case of ozone, MIRI's F1000W photometric filter may allow the 10 μ m bandpass to be accessed for a relatively small observing investment (verified with the JWST ETC¹ and APT), but the width of this filter will prevent an observation from measuring the bottom of a deep 10 μ m ozone feature. To elaborate, the width of the F1000W filter is fairly larger than that of the 10 μ m O₃ feature thus, an observation with this mode will include portions of the spectral continuum on either side of the feature and dilute the strength of the band and our sensitivity to it. For SO₂, the broad 16 – 22 μ m absorption feature may also be accessible with the F1800W, F2100W, or F2550W MIRI photometric filters, but the large 8.5 μ m absorption seen in emission is between two of MIRI's photometric filters (F770W and F1000W), so MIRI emission spectroscopy would be required. However, the large 7.3 μ m SO₂ feature may be accessible with the F770W photometric filter.

Emission spectroscopy of the full 5 – 14 μ m wavelength range, offered by MIRI LRS, would allow the observer to bin the data commensurate with the expected strength of the SO₂ 8.5 μ m feature, as well as the O₃ 10 μ m feature, simultaneously. Emission spectroscopy would also provide information on the strength of emission in the 10 – 14 μ m range, which may additionally probe the presence of trace SO₂ which tends to increase emission at these wavelengths. An emission observing campaign of this kind would be especially valuable for T-1c, which has already demonstrated a lower eclipse depth at 15 μ m than expected for an airless body (Zieba et al., 2023). T-1c additionally has 12.8 μ m unpublished MIRI photometric data.

¹<https://jwst.etc.stsci.edu/>

If this data showed increased emission at $12.8\mu\text{m}$ compared to the $15\mu\text{m}$ measurement, this would suggest either the presence of SO_2 or CO_2 , and follow-up observations targeting the 7.3 or $8.5\mu\text{m}$ SO_2 features would allow us to distinguish these two scenarios.

There are several potentially detectable transmission features for H_2O , CO_2 , CO , O_3 , and SO_2 found in the atmospheres modeled in this work, but they are presently below the sensitivity of publicly available transmission data (available for T-1b, c, d, and e; Espinoza et al., 2025; Glidden et al., 2025; Lim et al., 2023; Piaulet-Ghorayeb et al., 2025; Radica et al., 2025). Overall, the largest transmission features may be in the range of $75 - 100$ ppm, which is above the JWST noise floor of $5 - 50$ ppm (depending on the instrument; Bouwman et al., 2023; Lustig-Yaeger et al., 2023b; Rustamkulov et al., 2022; Seager et al., 2025), and therefore, once stellar noise is better handled and sufficient observing time is invested, these larger features may be accessible. Beginning with H_2O , three clear features at 1.4 , 1.9 , and $2.7\mu\text{m}$ are within the wavelength ranges of both NIRISS SOSS (used for T-1b and c; Lim et al., 2023; Radica et al., 2025) and NIRSpec PRISM (used for T-1d and e; Espinoza et al., 2025; Glidden et al., 2025; Piaulet-Ghorayeb et al., 2025), but these features are not detectable given the uncertainty on current data. Reducing this uncertainty could improve our ability to identify these H_2O features; however, H_2O is particularly problematic in transmission as it's also present in the stellar atmosphere (e.g., Wakeford et al., 2019). H_2O also produces an observable feature at $\sim 6\mu\text{m}$ in many of our atmospheres, but this would only be possible to access with MIRI. Although preliminary studies with MIRI show it may need a factor of 10 or larger observing investment to detect water compared to NIRSpec (Lustig-Yaeger et al., 2019a), the now known challenges of stellar contamination may suggest that this is a worthwhile investment if water detection on the TRAPPIST-1 planets is a community priority. The large $4.2\mu\text{m}$ CO_2 feature (particularly seen in our mixed CO_2 - CO and mixed O_2 - H_2O - CO_2 archetypes) is accessible to both NIRISS and NIRSpec spectroscopy though, similar to H_2O , more observations are needed in addition to current data to be sensitive to the feature size in our tenuous atmospheres. Although CO and O_3 provide features at $\sim 4.6\mu\text{m}$, these are also in the vicinity of strong CO_2 ($4.2\mu\text{m}$) and H_2O ($5 - 6\mu\text{m}$) absorption, and so they may be more difficult to retrieve. SO_2 is potentially detectable in transmission due to a trio of absorption features centered at $4\mu\text{m}$. Particularly, sharp absorption at $4.0\mu\text{m}$ could show the presence of SO_2 .

Future transmission observations of the system will have to address the presence of stellar contamination by developing and refining strategies to reliably remove stellar contamination. Rathcke et al. (2025) outlined a potential method for removing stellar contamination which involved observing back-to-back or overlapping transits of a target planet with T-1b, but this method relies on the assumption that T-1b is airless, which has been challenged by recent $12.8\mu\text{m}$ observations that indicated lower emission than expected (Ducrot et al., 2025). Acquiring additional out-of-transit baseline in future observing campaigns may also help to provide context on stellar activity around transits, and provide new data to calibrate models for removing stellar contamination. Moreover, we demonstrated in §3.3 how models may be positively or negatively correlated with transmission data. Given that the relative size of transmission features in our study are generally smaller than the size of uncertainty on data points, it would be expected that this correlation coefficient should be close to zero. While this is the case for some scenarios, T-1c in particular shows a strong negative correlation (~ -0.3) for all compositions, with dips below the spectral continuum coincident with the

locations of multiple water bands. This may indicate an over-removal of expected water contamination from the stellar atmosphere.

4.3.1 Implications for the Rocky Worlds DDT Time

The tenuous, outgassing sourced atmospheres and their spectral discriminants generated in this work may be broadly applicable to interpretation of observations other M dwarf terrestrial planets, if they are expected to follow similar evolutionary paths to those in the TRAPPIST-1 system. The joint JWST and Hubble Space Telescope (HST) Rocky Worlds DDT program (Redfield et al., 2024; Rocky Worlds DDT Program Website, 2025) will use MIRI photometry to observe the $15\mu\text{m}$ band of up to a dozen terrestrial exoplanets that orbit M dwarf stars. The archetype atmospheres in our work predict various absorption strength at the $15\mu\text{m}$ bandpass, ranging from strong in atmospheres containing significant CO_2 , to weak, particularly in dry O_2 -dominated atmospheres. Based on the $15\mu\text{m}$ data from the Rocky Worlds program, this work may be used to inform follow-up observations. Furthermore, we provide all of the temperature and mixing ratio profiles, as well as atmospheric spectra, generated through this work on GitHub. Spectra could quickly be recreated to represent Rocky Worlds targets given an alternative host star spectrum and planetary parameters using the temperature and mixing ratio profiles provided here.

4.4 Pressure-Temperature Profiles & Habitability

Observations of T-1d could provide an excellent test of the habitable zone concept (Kopparapu et al., 2013), as it sits within TRAPPIST-1’s optimistic habitable zone, but closer to the star than the conservative habitable zone’s inner limit (Gillon et al., 2017; Kopparapu et al., 2013). Existing simulations of T-1d’s possible climates have not converged on whether or not it is likely to be habitable, although many suggest either runaway states, or surface temperatures very much greater than 300 K, depending on atmospheric composition (Lincowski et al., 2018; Meadows et al., 2023; Turbet et al., 2020a, 2018; Wolf, 2017). However, a small subset of the existing simulations—which were performed for 1 bar or greater pressure atmospheres—were found to, at least for the current insolation, produce marginally habitable surface temperatures. These cases included dry O_2 -dominated atmospheres (Lincowski et al., 2018), or more modern-Earth-like scenarios, where the presence of reflective water clouds contributed to cooling (e.g., Meadows et al., 2023; Turbet et al., 2018). In contrast to previous simulations, the majority of our T-1d models sustain potentially Earth-like temperatures (273.15 – 300 K), but for atmospheric pressures that are < 1 bar. Our lower pressure atmospheres produce habitable temperatures even for atmospheres containing greenhouse gases such as our H_2O -dominated atmospheres, as well as our clear-sky CO_2/CO , although we note that these latter atmospheres are more likely to be desiccated. Overall these thinner atmospheres are conducive to cooling, and predict that surface temperatures for TRAPPIST-1 d will stay closer to its equilibrium temperature (~ 280 K for 0 albedo, ~ 260 K for an albedo of 0.3). For the higher pressure atmospheres (~ 1 bar) the dayside temperatures are seldom habitable, but habitable conditions are seen on the night side, especially for the mixed $\text{O}_2\text{-H}_2\text{O-CO}_2$ atmospheres, which are relatively Earth-like in composition.

The atmospheres our model found to be stable for T-1e are also quite thin (< 1 bar), which

leads to either colder climates that mostly fall within the ‘habitable snowball’ (242 – 273.15 K) temperature range, but with a smaller number in the Earth-like temperature regimes (273.15 – 300 K). In contrast, many previous studies find the Earth-like temperature regime to be common for T-1e models (e.g., [Fauchez et al., 2020](#); [Lincowski et al., 2018](#); [Meadows et al., 2023](#); [Sergeev et al., 2022](#); [Wolf, 2017](#)), although this can require the addition of greenhouse gas abundances, e.g. for CO₂ of several percent (e.g., [Meadows et al., 2023](#)). However, even in our models producing potentially ‘habitable snowball’ temperatures, many of our T-1e atmospheres possess pressures too low to exit the ‘gas’ phase of the water phase diagram (Figure 4.3). The compositions that fall squarely within the liquid region of the water phase diagram for T-1e are those atmospheres rich in the greenhouse gas CO₂, and with trace amounts of SO₂. [Turbet et al. \(2022\)](#) also reported colder to ‘habitable snowball’ global mean surface temperatures for dry planetary cases applied to T-1e (~215 – 245 K), which is similar to many of our models.

It is worth noting that the recent study by [Allen et al. \(2025\)](#) on JWST transmission data for T-1e highlighted the potential presence of CO in the atmospheric spectra. In this study, the mixed CO₂-CO atmospheres (the only case we show with detectable CO) provide the warmest surface temperatures for T-1e in our suite, particularly when also including trace SO₂. However, we find that nearly all of the T-1e models in our study fit the early transmission data for TRAPPIST-1 e ([Espinoza et al., 2025](#); [Glidden et al., 2025](#)) to $\leq 1\sigma$ (Figures 4.8 and 4.12). Consequently the data are currently unable to distinguish between our model predictions, but model outcomes may be distinguished or ruled out as further transmission data becomes available. Finally, we note that there are several cases where the globally-averaged nightside temperatures of models for T-1b and c fall within the liquid regime of the water phase diagram (Figure 4.3) and the Earth-like temperature region (273.15 – 300 K). Although the model used in this work has insufficient spatial resolution to map temperatures across the nightside and explicitly determine the nightside temperature minimum, which governs whether or not bulk components of the atmosphere can condense and collapse the atmosphere, the compositions modeled here are unlikely to collapse in these pressure-temperature regimes. For example, T-1c atmospheres in the liquid water regime have globally-averaged nightside temperatures between 250 and 550K, which is well above the <90K required to condense and collapse an O₂-dominated atmosphere ([Fray & Schmitt, 2009](#); [Turbet et al., 2018](#)). We also note that many of the atmospheres plotted in Figure 4.3 may have localized regions where liquid water is possible, as their day and night conditions span the liquid water region of the diagram.

For T-1f, g, and h we have modeled precipitation of water as ice, and find that when water is outgassed alone it is frozen before it can be photolyzed to produce O₂; however, if CO₂, an additional greenhouse gas, is outgassed along with water vapor, this can limit water ice formation. It is also worth noting that we began our simulations only with thin (0.1 bar) pressures of O₂, excluding any significant greenhouse gas — this was with the intention of testing whether secondary atmospheres can be fully generated from outgassing. While [Turbet et al. \(2020a, 2018\)](#) showed that CO₂ may freeze out on the outer TRAPPIST-1 planets, sufficient partial pressures of N₂ could help to prevent this.

4.5 Escape Flux Feasibility

An important caveat when interpreting results dependent on escape rates is that our atmospheric model does not consider ionization or ionized species, although this may not strongly impact our results, as neutral escape processes may still dominate. Non-thermal escape processes relying on the loss of ions (such as O^+ , O_2^+ , and CO_2^+) are expected to be quite high for rocky M-dwarf planets, such as those in the TRAPPIST-1 system (e.g. [Dong et al., 2018](#); [Li et al., 2025](#)). However, neutral escape processes are also expected to be considerable (e.g., Jeans, photochemical, etc) ([Gronoff et al., 2020](#)). For H_2 and H specifically, a diffusion-limited escape flux is calculated more rigorously, following previous work with the *Atmos* photochemical model (e.g. [Arney et al., 2016](#); [Lincowski et al., 2018](#)). For our other species, we do not consider ionization, or model the detailed physics of TOA escape, we instead approximate total escape processes with one TOA flux out of the atmosphere for any given escaping species considered (O , O_2 , CO_2). Total TOA escape fluxes are found by combining a fixed effusion velocity with the number density of the escaping species in the top layer of the atmosphere (detailed in Methods §2.4, Equation 2.25). While the escape rates found in the present study are higher than those in [Dong et al. \(2018\)](#), their MHD model captures only ion escape channels, whereas our effusion fluxes more closely represent neutral escape channels. Brain & Hinton (*priv. comm.*) find neutral escape from an exo-Mars (CO_2 -dominated) around Barnard’s Star (M dwarf) to be 1 – 3 orders of magnitude greater than ion escape. The findings of the present study show a similar trend for O_2 dominated atmospheres where our TOA escape flux (assumed to include neutral escape) may be up to 3 orders of magnitude greater than the pure ion escape rates for TRAPPIST-1 planets found by [Dong et al. \(2018\)](#).

The majority of our T-1b and c atmospheres that best fit emission data display oxygen escape rates that are relatively high ($\sim 10^{27} - 10^{30} \text{ s}^{-1}$) when compared to other values in the literature for TRAPPIST-1 ion escape ([Dong et al., 2018](#)) or solar system terrestrials ([Gronoff et al., 2020](#)), but this may be realistic. As illustrated by the grey regions in Figure 4.4, all of the T-1b and c models identified as $<3\sigma$ fits to the available emission data possess O_2 escape rates 1 – 3 orders of magnitude larger than the upper limit on O_2^+ escape rates provided by [Dong et al. \(2018\)](#) magnetohydrodynamic simulations. However, [Dong et al. \(2018\)](#) simulated O_2^+ escape from Venus-like (CO_2 -dominated) atmospheres, and in our O_2 -dominated atmospheres there is a higher concentration of O_2 available for escape at the exobase, increasing escape rates. The [Dong et al. \(2018\)](#) results also focus on ion escape, with reported expected escape rates on the order of $10^{26} - 10^{27} \text{ s}^{-1}$ for O^+ , and $10^{25} - 10^{26} \text{ s}^{-1}$ for both O_2^+ , and CO_2^+ . In contrast, our higher rates account for escape of neutral species, and as discussed above, neutral escape for planets orbiting M dwarfs, even for CO_2 atmospheres that likely have reduced oxygen escape rates, can be 1 – 3 orders of magnitude greater than that due to ion escape (Brain & Hinton, *priv. comm.*), suggesting that the literature’s simulated ion escape and our neutral escape rates are not inconsistent with each other.

In contrast to solar system bodies, which all generally have higher O escape than O_2 at present-day ([Gronoff et al., 2020](#)), the majority of our simulated atmospheres ($\sim 68\%$) exhibit higher O_2 escape rates than those for O . A possible explanation may be that the vast majority of stable atmospheres in this work are O_2 -dominated ($\sim 58\%$), so the larger concentration

of O_2 , when compared to O , may allow for higher escape rates. Furthermore there is some precedent in the solar system for O_2 loss rates to exceed that of O , occurring during certain events and time periods in the Martian atmosphere when the planet experienced heightened EUV due to solar winds or activity (Ma et al., 2004, 2018).

4.6 Chemical Disequilibrium False Positive Biosignatures on M Dwarf Planets

Following the method of Krissansen-Totton et al. (2016), we calculated the available Gibbs free energy for all the atmospheres generated in this study, and found that several atmospheres had values many times higher than Mars', especially for our CO -dominated atmospheres, although none were as high as Earth's. The Gibbs free energies for all the atmospheres in our study ranged from $<10^{-5}$ J/mol up to >800 J/mol in the most extreme cases. In Krissansen-Totton et al. (2016), it was shown that Venus, Earth including liquid water surface oceans, Earth without information on liquid water surface oceans, and Mars possess an available Gibbs free energy of 0.06, 2325.76, 1.5, and 136.35 J/mol, respectively. In general, atmospheres for planets closer to the star (T-1b, c, d, and, in some cases, e) in this study that include CO_2 outgassing tend to exceed the available Gibbs free energy of Mars. This is notable, as Mars exceeds the available Gibbs free energy of all solar system bodies, besides Earth when including its liquid water surface oceans (Krissansen-Totton et al., 2016). In our simulations the highest available Gibbs free energy was produced by T-1c's mixed CO_2 - CO atmospheres, at ~ 870 J/mol, which is over $7\times$ the available Gibbs free energy of Mars. These atmospheres therefore provide a specific example of an anomalously high chemical disequilibrium for an abiotic planet, a potential class of false positive biosignature previously described by Krissansen-Totton et al. (2016), possibly for planets with elevated levels of CO , O_2 , and H_2 driven by extreme UV radiation.

For the mixed CO_2 - CO atmospheres, those that are almost entirely CO have the lowest available Gibbs free energy of this archetype, and higher values are found for atmospheres with more equal amounts of CO_2 and CO , which enables more chemical reactions. In particular CO -dominated atmospheres have Gibbs free energies of $\lesssim 10^{-4}$ J/mol, while atmospheres with a closer to 50/50 split of CO_2 and CO can have Gibbs free energy values over 800. Based on our modeling results, we have found the balance of the following reactions is responsible for the disequilibrium in the mixed CO_2 - CO archetype:



This is in agreement with the results of Krissansen-Totton et al. (2016) for a Mars-like abundance of CO_2 and CO .

The mixed O_2 - H_2O - CO_2 atmospheres also produced a large range of Gibbs free energies (from 0.1 up to ~ 800 J/mol), and increases in available Gibbs free energy appeared to be tied to increasing CO_2 . The atmospheres displaying the highest Gibbs free energy possessing 70% to nearly 100% CO_2 . Upon further investigation, disequilibrium in these CO_2 atmospheres can either be caused by the trace presence (100 ppm) of CO , and the reactions given in equation 4.1, or by the balance of O_2 , H_2O , and CO_2 . However, this latter combination of

gas abundances is dictated by the photolysis rates of water, as well as the 2 and 3-body reactions that deplete O_2 in favor of atomic O and OH, and it is difficult to identify which reactions dominate the disequilibrium.

While the abiotic mixed CO_2 -CO archetypes can generate high available Gibbs free energies (>800 J/mol for T-1c) and could potentially be interpreted as false-positive chemical disequilibrium biosignatures, placing an accurate constraint on the Gibbs free energy via observation would be extremely difficult. If CO is not accessible in the observed wavelength range, or is hard to detect or distinguish (see §4.3), the inferred Gibbs free energy values can drop significantly from this high Gibbs free energy case. If O_3 (potentially found at $\sim 4.7\mu\text{m}$), rather than CO, was believed to be present in the atmosphere with CO_2 , the interpretation may favor a mixed O_2 - H_2O - CO_2 composition which, for T-1c, only possesses an available Gibbs free energy of ~ 0.4 J/mol (without SO_2), rather than the >800 J/mol possible for a mixed CO_2 -CO atmosphere.

However, if a mixed CO_2 -CO atmosphere with an >800 J/mol Gibbs free energy was confidently detected, it may still be possible to identify it as a false-positive detection, and not a disequilibrium mediated by biology. First, confirmation of CO_2 , CO, and O_2 together at substantial levels in the atmosphere may provide a clue that CO_2 outgassing and subsequent photolysis driven by incident stellar UV is responsible for the disequilibrium, as CO and O_2 are daughter products of CO_2 photolysis and are more likely to exist together in a desiccated and uninhabitable atmosphere (Gao et al., 2015; Meadows, 2017; Schwieterman et al., 2016). Moreover, the lack of CH_4 in the atmosphere may further indicate that the disequilibrium is abiotic because the high fractions of oxygenated species in the atmosphere are likely to destroy CH_4 produced by a non-biological processes such as volcanism and serpentinization (Domagal-Goldman et al., 2014). The maximum fluxes of CH_4 from these abiotic processes are much lower than biological generation on our planet (Guzmán-Marmolejo et al., 2013).

4.7 Study Limitations

In this work, we have provided an initial exploration of where the balance of photochemical, climate, outgassing, and atmospheric loss processes may support tenuous secondary atmospheres on the TRAPPIST-1 planets; however, there are several limitations of this work that should be noted when interpreting the results shown here, most notably due to our incomplete sampling of possible outcomes, and the limited number of outgassed species considered. Importantly, we have not explored a statistically sized sample of the phase space defined by the ranges of outgassing and escape processes. Because of this sampling limitation, we cannot quantify statistical likelihoods that the planets possess an atmosphere, or make any predictions as to their most likely compositions. We can instead say that we have identified cases where specific atmospheres and compositional archetypes are plausible within the phase space. However, there may be boundary combinations that we did not test that could lead to compositions that are missing in our results for particular planets. Input combinations that were not explored also have the potential to lead to spectral features of varying strength and detectability compared to the sample of spectra given here. For example, an O_2 -dominated atmosphere that has less water than the sample set in this work could lead to a larger ozone contribution and a deeper, and potentially more observable, feature at $10\mu\text{m}$.

One particular difficulty in applying a statistical sampling method to a study of this nature is the computation time required by each of the model components, particularly climate. As a part of one *VPL Climate* simulation, a full line-by-line radiative transfer solution is calculated around $2 - 3\times$ on average, and a climate simulation may need to be run many times before it is converged. In total, some atmospheres may take multiple days to achieve global convergence. Future work could explore ways to improve computational efficiency, and provide a more comprehensive sample of the diversity of plausible atmospheres.

In the particular case of T-1f, which had a notably lower number of stable atmospheres than the other planets in this study (Table 4.1), many of the atmospheric input combinations tested failed to achieve global convergence. This is a state when, on a single pass through all of the photochemical, surface pressure, and climate models, the climate model finds local convergence on the first attempt and the surface pressure never changes by more than 3%. In the case of T-1f, many simulations were not able to find local climate convergence on the first attempt in one pass through the global model. Our convergence strategy was very strict, as oscillations in the temperature profile of the uppermost atmospheric layers can prevent local climate convergence, even when the bulk atmosphere is not changing considerably. Future work could explore a more sophisticated scheme for convergence checking within the climate model that takes each individual atmospheric layer into consideration, as opposed to the global average used in this project. A more advanced convergence method may identify a larger sample of stable atmospheres for all planets in this study.

Another limitation to note is that the array of gases we considered as outgassed or escaping species (H_2O , CO_2 , and their daughter products) is likely a subset of the species that could be present. For example, from solar system terrestrials we know other constituents may be outgassed including CH_4 , sulfur-bearing species, or chlorine-bearing species (e.g., Gaillard et al., 2021; Redwing et al., 2022). There may be many more possible compositions for these planetary atmospheres when considering more complex outgassing compositions, that were not explored in the present study. Similarly, our treatment of atmospheric sinks (e.g., deposition and escape) was simple, assuming some flux out of the bottom or top of the atmosphere. Future work may look into coupling our simulations to more advanced models of escape or surface-atmosphere exchange. Finally, while we did consider a separated day and night side climate calculation for the interior planets, we did not have the capability to model water condensation and atmospheric collapse on the nightside that may be expected on tidally locked planets and could be another pathway to complete atmospheric erosion (Turbet et al., 2020a, 2018).

Clouds, dust, and hazes also constitute an area of potential uncertainty, as these influence planetary climate and can modify atmospheric spectra. However, due to the low surface pressures and dry compositions seen across the majority of our models, clouds may only have a minimal effect on the spectra presented here. In general, at the low pressures exhibited by the majority of our stable atmosphere outcomes, diffusive and convective mixing become weaker, which are necessary processes for gas replenishment and cloud growth (Helling, 2019), suggesting that significant cloud formation is unlikely in these atmospheres. In terms of Earth-like water clouds, we tracked the condensation of H_2O in our models and found no evidence for this on T-1b through d. H_2SO_4 also does not condense on T-1b (Lincowski et al., 2018). Water did condense on T-1e and the outer planets in the system, but for T-1f through h this often led directly to permanent loss of water from the atmosphere, and atmospheric

collapse in the H_2O only outgassing cases. Thus, T-1e may have the highest potential in our model to form water clouds. However, even if clouds do successfully form, they may have very little impact on the predicted transmission spectra for many of our modeled outcomes. Looking at the formation of sulfuric acid clouds in Venus-Like high pressure CO_2 -atmospheres for the TRAPPIST-1 planets, [Lustig-Yaeger et al. \(2019b\)](#) showed that H_2SO_4 clouds would truncate T-1c and d transmission at altitudes near 0.01-0.001 bars and T-1e transmission spectra at about 0.01 bars, which has the potential to affect the smaller fraction of our model outcomes that have higher surface pressures than this. However, given that sulfuric acid cloud formation occurs at lower altitudes for planets further from the star, [Lustig-Yaeger et al. \(2019b\)](#) showed that the clouds formed at pressures above the limiting opacity of the atmosphere itself for planets beyond the orbit of T-1e, resulting in the effect of the clouds essentially being invisible, which produced a strong match between their cloudy and clear-sky spectra ([Lustig-Yaeger et al., 2019b](#)). They also showed that emission spectra may be more robust against influence from clouds than transmission observations ([Lustig-Yaeger et al., 2019b](#)). In general, while the addition of clouds may perturb the climate and/or transmission spectra of a subset of the higher surface pressure atmospheres in this study, we have focused on presenting valid clear-sky solutions for the lower pressure atmospheres that are so far a better fit to T-1b and c data ([Greene et al., 2023](#); [Ih et al., 2023](#); [Lincowski et al., 2023](#); [Zieba et al., 2023](#)), and we will leave cloud modeling for future work.

Dust and hazes are likely more influential than clouds for the low pressure regime of many of our atmospheric models. Dust in particular provides a large source of uncertainty, as comparisons with Mars indicate that absorption features caused by dust can overlap spectroscopically with the regions of interest in this work ([Bandfield et al., 2003](#); [Erard et al., 1994](#)). Dust may be more important for reflected light spectra, which we do not present here, but will be of interest for the upcoming Habitable Worlds Observatory. Hazes additionally may be present on these planets, but the formation of organic hazes requires the presence of methane ([Arney et al., 2016](#); [Turbet et al., 2020a](#)) which is not considered in our atmospheric models. Hazy methane atmospheres may also be valid solutions for the TRAPPIST-1 planets, but are not the focus of this study. Future work could consider the effect of dust, hazes, and clouds on climate and atmospheric spectra for tenuous atmospheres on the TRAPPIST-1 planets.

5 Conclusions

We have conducted self-consistent photochemical-climate calculations for terrestrial exoplanets orbiting TRAPPIST-1, across a range of outgassing and escape processes, and shown that the high expected atmospheric escape rates do not preclude tenuous atmospheres that may be consistent with current JWST data. Our model is the first to couple the processes of climate, photochemistry, outgassing and escape, and account for variable surface pressures as these atmospheres evolve towards model equilibrium. Through plausible water and/or CO_2 outgassing rates constrained for these planets by [Thomas et al. \(2025\)](#), modified by photochemistry and balanced by escape, we demonstrate that an array of atmospheric compositions may arise in the system including steam, dry or wet O_2 , mixed CO_2 - CO , and mixed O_2 - H_2O - CO_2 . Most commonly, our stable atmospheres have 0.1 mbar – 1 bar surface pres-

tures, and exhibit a range of surface temperatures from 100 – 580K. For T-1 d and e, we find several stable atmospheres with globally-averaged temperature and pressure combinations that permit liquid surface water. We also find similar potentially habitable conditions for the hemispherically-averaged nightsides of TRAPPIST-1 b and c.

Our atmospheres present relatively large spectral features in transmission, even for some 0.05 bar terrestrial atmospheres ($\lesssim 150$ ppm) but are still typically smaller than the uncertainty associated with JWST transmission data from the system to date ($\pm >100$ ppm; Allen et al., 2025; Espinoza et al., 2025; Glidden et al., 2025; Lim et al., 2023; Radica et al., 2025), indicating that we do not currently have the sensitivity to distinguish or rule out these atmospheres to reasonable confidence ($>3\sigma$) in transmission. Conversely, emission data available for T-1b and c provides more robust measurements, though limited to only one or two wavelengths (12.8 or $15\mu\text{m}$). Comparison to emission observations suggests that extremely thin (~ 0.01 bar) dry O_2 -dominated compositions without significant CO_2 may provide the best atmospheric match to the current emission data for T-1b ($<3\sigma$; Ducrot et al., 2025; Gillon et al., 2026; Greene et al., 2023). In contrast, the best atmospheric fits found for the T-1c emission data ($<1\sigma$; Gillon et al., 2026; Zieba et al., 2023) are from slightly thicker O_2 -dominated atmospheres (≤ 0.3 bars) with trace fractions of greenhouse gases, though higher fractions of greenhouse gases are equally plausible if the atmospheric pressures are lower. Given the low pressures in our models, even some atmospheres with up to $\sim 20\%$ CO_2 cannot be ruled out unambiguously by $15\mu\text{m}$ data alone for T-1c if sufficient water ($\sim 10\%$) is also present to heat the atmosphere.

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7 Chapter Appendix

7.1 Correlation Coefficient Proof of Concept

Here we provide a simple example that illustrates how a model can be preferred over another using the Pearson Correlation Coefficient (PCC) when they both report the same χ^2 value. Figure 4.15 illustrates the example we will describe here. Consider a set of observations with associated uncertainty (black diamond points connected by dashed lines, Figure 4.15),

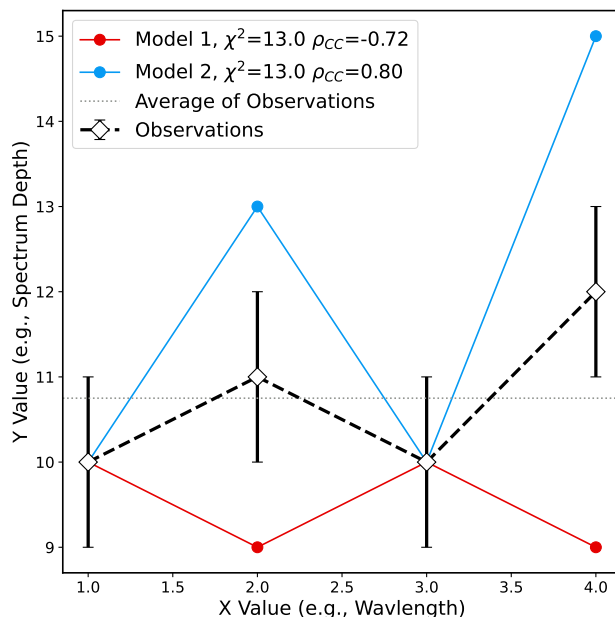


Figure 4.15: An example dataset (black points connected by dashed line) compared to two models (red and blue lines). The average of the observations is shown by the dotted grey line to allow better by-eye comparisons. While the models both display the same χ^2 fit (13 in this case), model 1 and 2 are strongly negatively and positively correlated, respectively, suggesting model 2 may be a better overall fit if this example is taken to represent transmission spectra.

which could be transmission points at specific wavelengths. We want to compare two different models (blue and red lines, figure 4.15) to the data, but the two models produce the same χ^2 goodness of fit metric (13 in this example), and thus the same p -value and σ fit.

While the χ^2 goodness of fit test cannot show preference for one model over the other in this example, the PCC can provide more information. For model 1 (red line, Figure 4.15) the PCC is -0.72, while model 2 (blue line, Figure 4.15) has a PCC of 0.8, indicating that model 1 is very strongly *negatively* correlated with the observations and model 2 is very strongly *positively* correlated. In the physical example of a transmission spectrum as a function of wavelength, this may be interpreted as model 2 exhibiting absorption features when there is stronger absorption in the dataset. Therefore, one may conclude in this example that model 2 has the correct absorbers present, albeit too strongly, while model 1 is missing key features that would allow it to match the data.

CHAPTER 5

USING BAYESIAN NESTED SAMPLING TO CONSTRAIN OUTGASSING, ESCAPE RATES, AND PLAUSIBLE ATMOSPHERIC COMPOSITIONS FOR TRAPPIST-1C

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1 Summary

Upcoming NASA missions, such as the Habitable Worlds Observatory, aim to detect alien life via atmospheric biosignatures on Earth-like exoplanets. However, constraining atmospheric species abundance alone is insufficient for biosignature detection because the source flux of a given species is the true indicator of biogenic production, as demonstrated by many gases in Earth’s atmosphere. Furthermore, abiotic tenuous secondary atmospheres must be generated and maintained by replenishment processes balancing expected atmospheric escape, particularly for M dwarf planets which are subjected to heightened XUV radiation and stellar activity. The irradiated TRAPPIST-1c is an excellent example of a hot terrestrial planet that has been found to be likely airless, or posses a very tenuous atmosphere. Here we use a photochemical model with realistic climate profiles as the forward model to a retrieval-style Bayesian inference framework that targets constraints on outgassing and escape boundary conditions that generate atmospheres best matching the emission data for TRAPPIST-1c. We show that the most likely atmospheric solutions for the planet are thin ($\sim 1 \text{ mbar} - 0.5 \text{ bar}$) O_2 -dominated atmospheres with $1 - 10\%$ water at the surface, that may or may not contain detectable trace CO_2 . Furthermore, we explore how this framework can suggest constraints on geochemical properties of the planetary interior. Finally, we discuss future observational discriminants for TRAPPIST-1c, and find that ozone may be the best candidate for follow-up observations targeting thin oxygen atmospheres.

2 Brief Introduction

In this chapter, we use Bayesian nested sampling (via the *MultiNest* algorithm; Buchner et al., 2014; Feroz et al., 2009, 2019) to define the probability of sampled outgassing and atmospheric escape rates to generate atmospheres that match the T-1c emission data (Gillon et al., 2026; Zieba et al., 2023) when considering our forward model. After completing the nested sampling process, we analyze the resulting posterior probabilities, explore ways to extract unique solution sets, and consider the highest likelihood atmospheric models found in our phase space. As future observing campaigns provide better spectral constraints on T-1c or even other terrestrial exoplanets of interest, we anticipate that the method demonstrated here will be valuable in identifying likely atmospheric compositions and connecting observations to possible geologic sources and sinks.

In the next section, we present the posterior probabilities generated by our inference framework (§3.1), provide convergence assessments (§3.1.1), and explore methods to pull out a discrete solution set (§3.2 and §3.3). From our identified solution sets, we consider the photochemical and spectral profiles of likely atmospheres and determine if different boundary condition sets lead to observationally distinct atmospheres. Furthermore, how the preferences for outgassing rates found in this study may inform properties of the planetary interior when

considering the work of [Thomas et al. \(2025\)](#) (§3.4). We discuss the photochemical and spectral behavior of our atmospheric solutions, future observational discriminants, and the study limitations in §4. Finally we conclude in §5.

3 Results

Using ellipsoidal Bayesian nested sampling with *MultiNest* ([Buchner et al., 2014](#); [Feroz et al., 2009](#)) applied to emission measurements for T-1c ([Gillon et al., 2026](#); [Zieba et al., 2023](#)), we have constrained the posterior probabilities of 7 input surface and top of atmosphere boundary conditions that govern the formation, maintenance and composition of the atmosphere. The inputs we consider are H₂O outgassing flux, CO₂ outgassing flux, O effusion velocity (top-of-atmosphere, TOA, escape), O₂ effusion velocity, CO₂ effusion velocity, CO deposition velocity (loss at the surface), and trace fixed surface SO₂ mixing ratio. We first present the constrained posteriors and conduct cross-validation to provide insight into how well sampled the phase space is (§3.1). We then use two approaches to identify the most likely atmospheric solutions, across the phase space of atmospheres that can be generated with our considered sources and sinks, that match the T-1c emission data. First, we present the highest likelihood samples found by *MultiNest*, which we defined as the top 10% of posterior samples ranked by log-likelihood (§3.2). Next, for the equally weighted samples reported by *MultiNest*, we use a Gaussian Mixture Model (GMM) to identify clusters of samples in the 7D phase space, ultimately presenting 8 different solutions with associated uncertainty (§3.3) found through the solution set identification method described in §2.3.2. For every atmospheric solution considered, we present the photochemical profiles and atmospheric spectra that were modeled.

3.1 Posterior Inference

MultiNest was run until it achieved an evidence tolerance of 10, which led to over 11500 calls of the forward model, and ultimately producing a set of 1125 equal-weighted posterior samples. The evidence tolerance of 10 was chosen because our analysis does not require precise Bayesian evidence estimation for multiple forward model comparison, we are solely interested in characterizing the posterior distribution of atmospheric boundary parameters based on our single forward model framework. At this tolerance, the resulting posterior samples are sufficient for the inference goals of this work, which are to characterize the posterior probabilities of the input atmospheric boundary conditions to generate atmospheres that match the T-1c emission data ([Gillon et al., 2026](#); [Zieba et al., 2023](#)). The adequacy of the sampling is further quantified through cross-validation (§3.1.1). We acknowledge that a stricter tolerance would yield a more finely resolved posterior, but the computational cost of the forward model made this impractical. Given the consistency found across the atmospheres in our solution sets (§3.2 and §3.3), we conclude that the addition of further sampling would not change our results significantly.

Figure 5.1 shows a corners plot of the posterior probability distributions for the atmospheric boundary conditions constrained in this project. The corners plot shows that there was a preference for the H₂O and CO₂ outgassing fluxes, the trace mixing ratio of SO₂

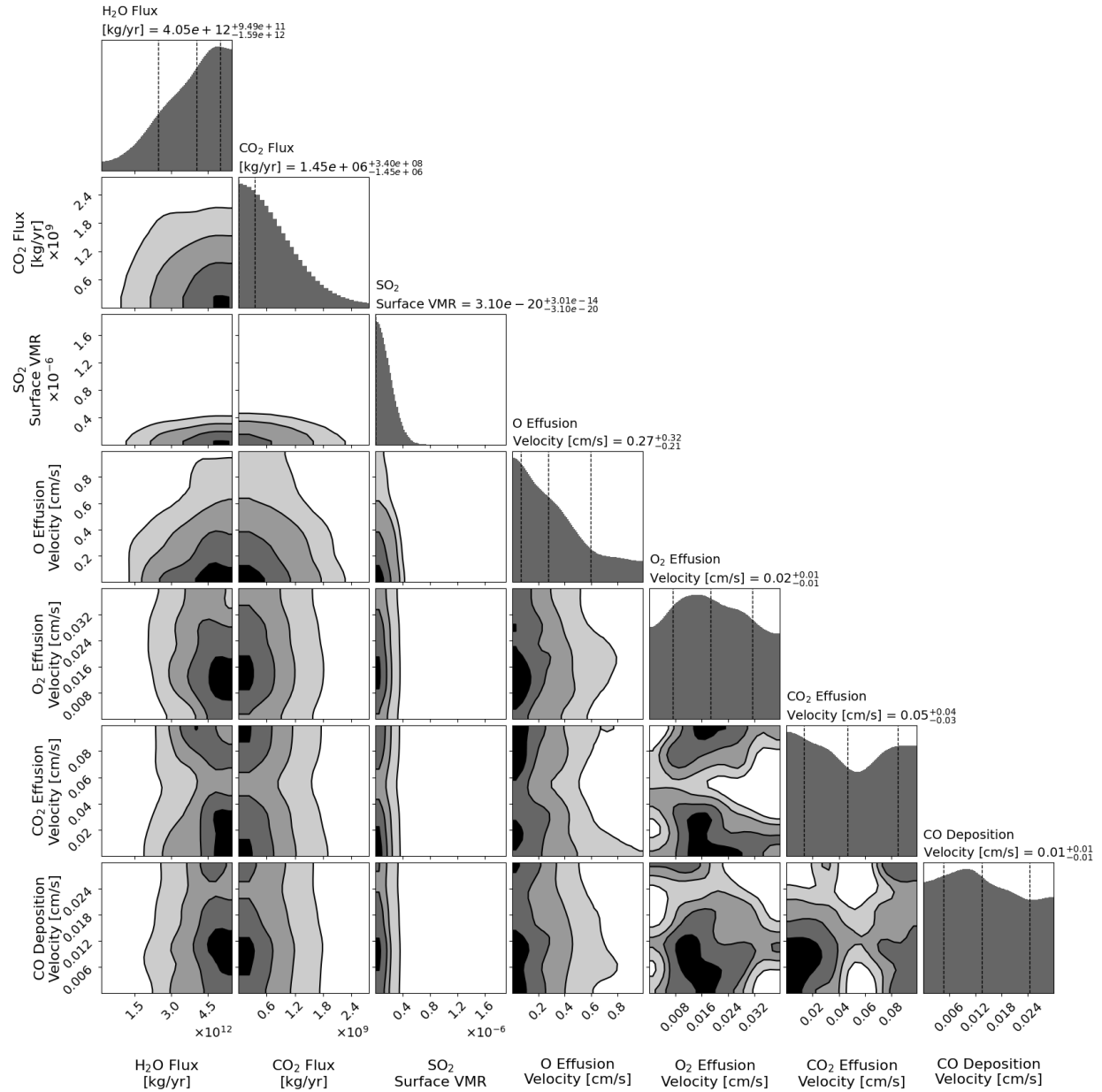


Figure 5.1: Posterior probability distributions constrained by our Bayesian inference pipeline for all 7 input parameters. From left to right and top to bottom, the parameters are H₂O outgassing flux [kg/yr], CO₂ outgassing flux [kg/yr], O effusion velocity (top-of-atmosphere, TOA, escape) [cm/s], O₂ effusion velocity [cm/s], CO₂ effusion velocity [cm/s], CO deposition velocity (loss at the surface) [cm/s], and trace fixed surface SO₂ mixing ratio.

Kernel	RMSE	R ² Value
Radial Basis Function (RBF)	0.67	0.55
Matérn 1.5	0.58	0.66
Matérn 2.5	0.60	0.63
Rational Quadratic	0.53	0.72
Rational Quadratic + Matérn 1.5	0.54	0.71

Table 5.1: The performance of all five tested Gaussian Process (GP) kernels during the cross-validation analysis, which tests the completeness of the posterior probability and the ability to predict probability values based on the dataset. The rational quadratic kernel (bolded) minimizes the root mean squared error (RMSE) and maximizes the R² value, indicating that the best performing kernel’s predictions are half a standard deviation away from the true posterior (on average) and that $\sim 70\%$ of the variance in the posterior can be explained by the GP.

injected, and the O effusion velocity, but the O₂ and CO₂ effusion velocities and the CO deposition velocity remain relatively unconstrained. There is a strong preference for higher H₂O outgassing rates, which was also found in [Gialluca et al. \(2026, In Review\)](#), though not in a statistically robust way. The preference for sources of CO₂ and SO₂ follows an opposite trend, with smaller levels of these constituents preferred. Similarly, low O effusion velocities were preferred.

3.1.1 Cross-Validation

To evaluate how well-constrained the posterior probabilities are across our parameter space, we perform a cross-validated Gaussian Process (GP) regression, testing whether a GP can accurately learn and generalize posterior values from a set of training points. We tested the performance of five different GP kernels to predict posterior values: a Radial Basis Function (RBF), Matérn 1.5 (once differentiable), Matérn 2.5 (twice differentiable), Rational Quadratic, and a Rational Quadratic plus Matérn 1.5 sum kernel. The root mean squared error (RMSE) and R² value found for each kernel is shown in Table 5.1. Given the log-transformation, zero mean and unit variance normalization preprocessing of the posterior dataset, an RMSE of 1 would indicate that GP predictions are exactly 1 standard deviation away from the true posterior values of the testing set. The best performing GP used the rational quadratic kernel, reporting an RMSE of 0.53 and an R² value of 0.72. The RMSE indicates that the GP’s predictions were, on average, half a standard deviation away from the true posterior, and overall the R² indicated that $\sim 70\%$ of the variance in the posterior can be explained by the GP.

Highest-Likelihood Solution Set Info

H ₂ O Flux (kg/yr)	$2.18 \times 10^{12} - 5.42 \times 10^{12}$
CO ₂ Flux (kg/yr)	<i>Negligible</i> – 1.33×10^7
SO ₂ Trace Surface Mixing Ratio	$1.02 \times 10^{-20} - 9.87 \times 10^{-15}$
O V_{eff} (cm/s)	0.012 – 0.80
O ₂ V_{eff} (cm/s)	$6.10 \times 10^{-4} - 3.16 \times 10^{-5}$
CO ₂ V_{eff} (cm/s)	0.0025 – 0.10
CO V_{dep} (cm/s)	$7.45 \times 10^{-4} - 0.030$
Fit to Emission Data (σ)	0.079 – 0.12
Combined Fit to Transmission & Emission Data (σ)	1.91 – 2.38

Table 5.2: The ranges for all seven input dimensions (top 7 rows), fit to emission data (8th row), and combined fit to transmission and emission data (last row) of the Highest-Likelihood solution set samples.

3.2 Highest-Likelihood Solution Set

The Highest-Likelihood (HL) Solution Set is the top 10% of *MultiNest* equal-weight posterior samples ranked by log-likelihood. Out of 1125 equal-weight posterior samples, this likelihood criteria led to 48 unique samples in the HL set. Table 5.2 provides the range of input values found across the HL set, as well as their range of fits to the T-1c emission data (Gillon et al., 2026; Zieba et al., 2023) and combined fits to all available T-1c data (including transmission; Radica et al., 2025). Note that Bayesian inference was conducted to maximize the fit to emission data only (as it is more robust against stellar contamination issues; Rackham et al., 2018).

Figure 5.2 shows the adopted pressure-temperature profiles and modeled gas mixing ratio profiles of the 48 samples in the HL solution set; their derived surface pressures range from 0.07 to 0.44 bars. All samples in the HL set are oxygen (O₂) dominated with $\sim 87 - 99\%$ at the surface. The second most abundant molecule near the surface in these atmospheres is H₂O, with between approximately a few percent up to nearly 15% at the surface. Ozone ranges from approximately 0.1 to 10 ppm at the surface. At the top of the atmosphere, all models become dominated by atomic oxygen as photolysis strengthens. In general, the altitude profiles of H₂O, O₂, O₃, and atomic O remain very consistent across samples in

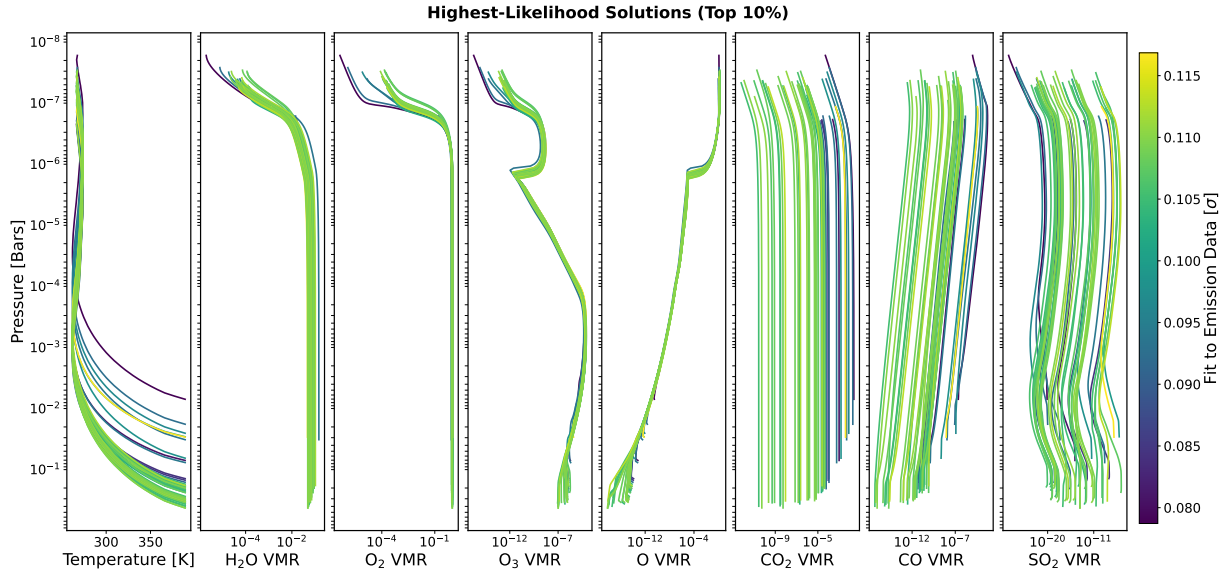


Figure 5.2: From left to right, the pressure-temperature profile and H_2O , O_2 , O_3 , O , CO_2 , CO , and SO_2 volume mixing ratio profiles for the HL solution set. Samples are colored by their σ fit to the T-1c emission data (Gillon et al., 2026; Zieba et al., 2023), which is generally $\sim 0.1\sigma$. H_2O , O_2 , O_3 , and O profiles remain nearly identical across samples in this set, but the carbon-bearing species show more variation.

the HL set. In contrast, CO_2 , CO , and SO_2 vary more across the HL samples, though they generally comprise a considerably smaller fraction of the atmosphere than oxygen or water. Across the HL set, CO_2 ranges from ~ 0.3 ppb up to nearly 3% at the surface, which is inversely proportional to the surface pressure — that is, when surface pressure is smaller, CO_2 tends to be larger. Since CO_2 photolysis is the primary source of CO , the amount of CO in the atmosphere increases with CO_2 and ranges from $\sim 5 \times 10^{-8}$ up to 225 ppb.

Figure 5.3 shows the transmission spectra (top row), day-side emission spectra (bottom left), and night-side emission at $15\mu\text{m}$ (bottom right) for the samples in the HL solution set. Additionally, Figure 5.4 provides an example spectrum pulled from the HL solution set colored by molecule absorption to illustrate what is causing various spectral features; we find that the spectral features across every solution presented here match the same pattern shown by Figure 5.4, though with varying strength. H_2O features can primarily be seen across the transmission spectra particularly between $1 - 3.5\mu\text{m}$ and centered at $6.3\mu\text{m}$. Ozone can also be seen in transmission, particularly at $0.6\mu\text{m}$ and $4.7\mu\text{m}$. The $4.2\mu\text{m}$ CO_2 transmission feature may also be present, though with varying strength depending on the exact solution. In emission, there is a clear ozone feature at $9.6\mu\text{m}$, and CO_2 absorption with varying strength at $15\mu\text{m}$. To achieve the band depth at $15\mu\text{m}$ observed with JWST, the atmospheres in this set either have low pressure with higher CO_2 (leading to a feature at $15\mu\text{m}$ in the spectrum) or higher pressure with less CO_2 (leading to an overall depressed continuum near $15\mu\text{m}$). Finally note that H_2O absorption also appears in emission at wavelengths shorter than $\sim 9\mu\text{m}$.

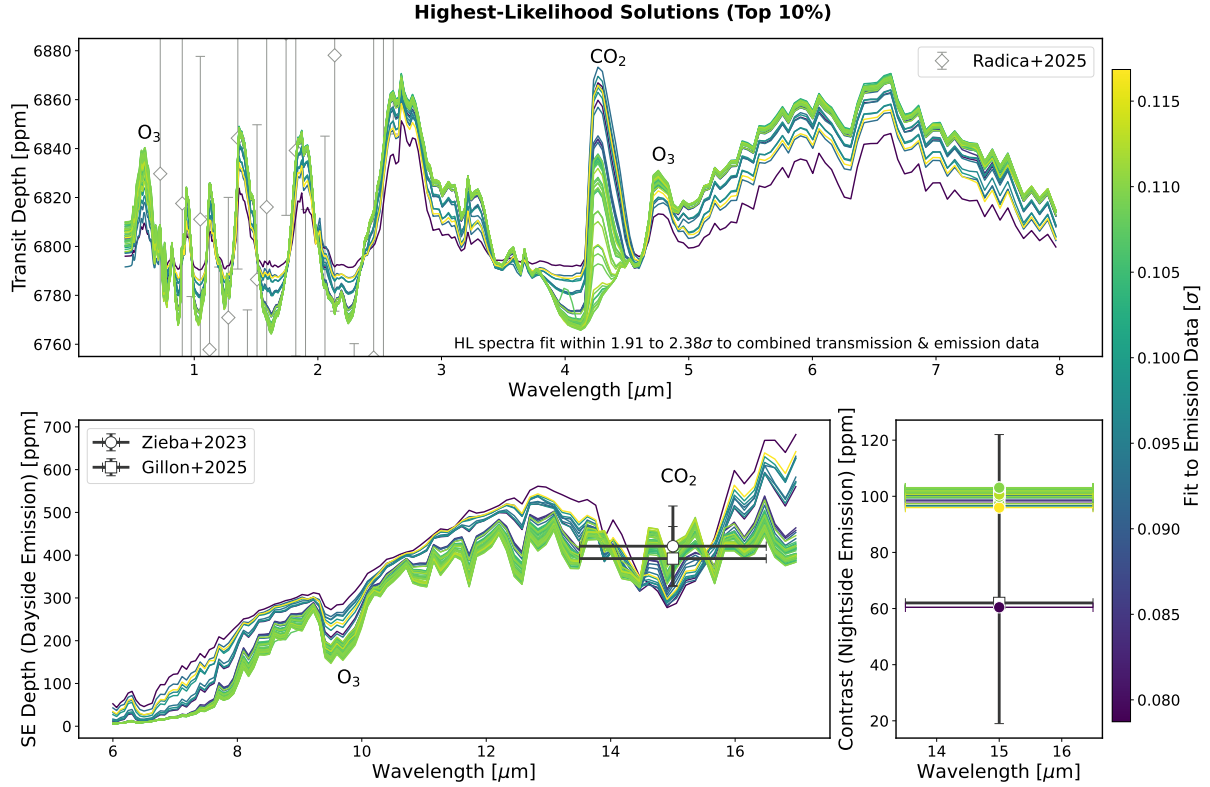


Figure 5.3: The transmission spectra (top row), day-side emission spectra (bottom left), and night-side emission in the JWST MIRI F1500W $15\mu\text{m}$ bandpass (bottom right) for the samples in the HL solution set. Transmission (Radica et al., 2025) and emission (Gillon et al., 2026; Zieba et al., 2023) JWST observations are also plotted for comparison. Spectra are colored by their fit to the emission data only, as this was the metric used by the Bayesian inference model. However, spectra were found to fit to all observational data between $1.91 - 2.38\sigma$ when including transmission. Features that may be caused by O_3 or CO_2 are labeled, and all other unlabeled spectral features may be attributed to water.

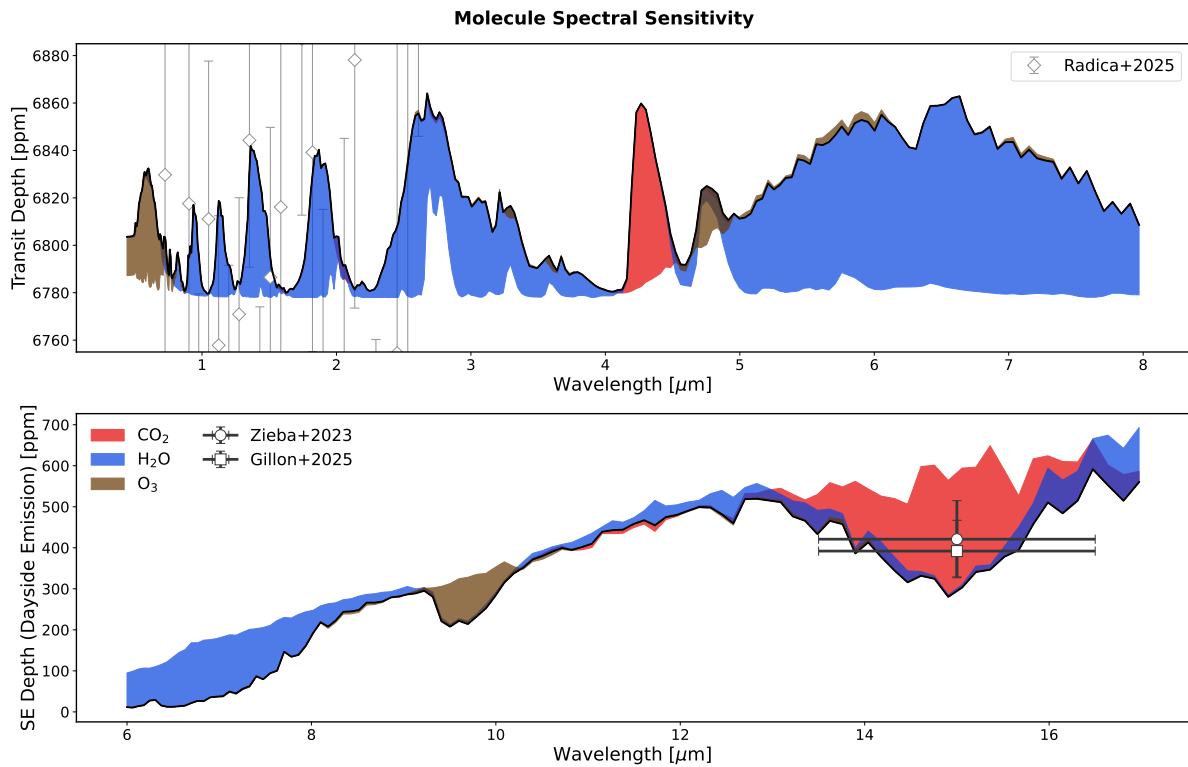


Figure 5.4: Example T-1c transmission (top) and emission (bottom) spectra colored by the contribution of atmospheric molecules. Spectral features for the atmospheres in our solution sets are dominated by H_2O , CO_2 , and O_3 activity.

3.3 Cluster Solutions

When fitting Gaussian Mixture Models (GMMs) across 380 random initializations, minimization of the Bayesian Information Criterion (BIC) most frequently identified 9 components (i.e., ‘clusters’ or ‘solutions’) as the optimal partitioning of the posterior samples. Specifically, 138/380 or 36% of random states led to a 9 component solution set, whereas the next best number was an 11 component set selected by 62/380 or 16% of random states. None of the random states led to solutions less than 7 or greater than 12 components. In general, the exact number of optimal solutions can fluctuate particularly due to outlying simulations or sparsely sampled regions of the posterior. We select seed 289 as the reported solution set, which was most closely aligned the average of all random states with a 9 component solution sets (selected through a Euclidean distance minimization). Additionally, upon further evaluation we found that solution 9 often only contained a few unique samples (2 for seed 289), suggesting that there were a few outlier cases that the model could not assign to larger clusters. Because of this, we remove solution 9 from the final set and continue the analysis only with solutions 1 through 8.

Figure 5.5 shows a corners-style plot with 2D error bars for every pair of input parameters for each of the 8 solutions. In general every solution is tightly located in water and CO₂ outgassing flux, though the latter has much larger error bars (spanning multiple orders of magnitude). The largest variation between solutions is seen in the effusion velocities, particularly O₂ and CO₂.

Figure 5.6 shows the median and 1σ ranges of the pressure-temperature profile and H₂O, O₂, O₃, O, CO₂, CO, and SO₂ volume mixing ratio profiles of the 8 solutions from the GMM cluster analysis. Similarly to the HL solutions, the water, O₂, O₃, and atomic O profiles remain tightly constrained across all solutions. There is larger uncertainty in the profiles of CO₂, CO, and SO₂, those these all remain trace constituents compared to the bulk oxygen species. Finally note that the presence of an upper atmosphere temperature inversion is generally unconstrained, as the resulting atmospheric compositions were not significantly affected.

Figures 5.7 and 5.8 show the median and 1σ range of the 8 GMM solutions’ transmission and emission spectra, respectively. The emission spectra also include emission in the 15 μ m MIRI F1500W bandpass to compare with nightside observations from Gillon et al. (2026). All spectra match within 1σ and generally match to the HL set as well. Transmission is dominated by water features, but ozone (at 0.6 μ m and 4.7 μ m) and CO₂ (at 4.2 μ m) can also be seen with varying strength. In emission, the strength of CO₂ absorption at 15 μ m and SO₂ near 7 μ m also varies between solutions, but not significantly outside of the 1σ uncertainty region. Notably, every solution has a 9.6 μ m absorption feature, which was absent in the CO₂-poor runs of Gialluca et al. (2026, In Review). Finally, the fit of all GMM solutions to the T-1c emission data (Gillon et al., 2026; Zieba et al., 2023) only and to the combined emission and transmission (Radica et al., 2025) data is shown in Figure 5.9. All GMM solutions fit to $\sim 0.2 - 2\sigma$, considering uncertainty on measurements. When including transmission, the GMM solutions fit all current T-1c data to $\sim 2 - 2.5\sigma$. Note, however, that a joint fit to emission and transmission data is more heavily weighted toward the transmission spectrum. This is because the χ^2 calculation weights each data point equally, and although the transmission data were collected in a single observing campaign,

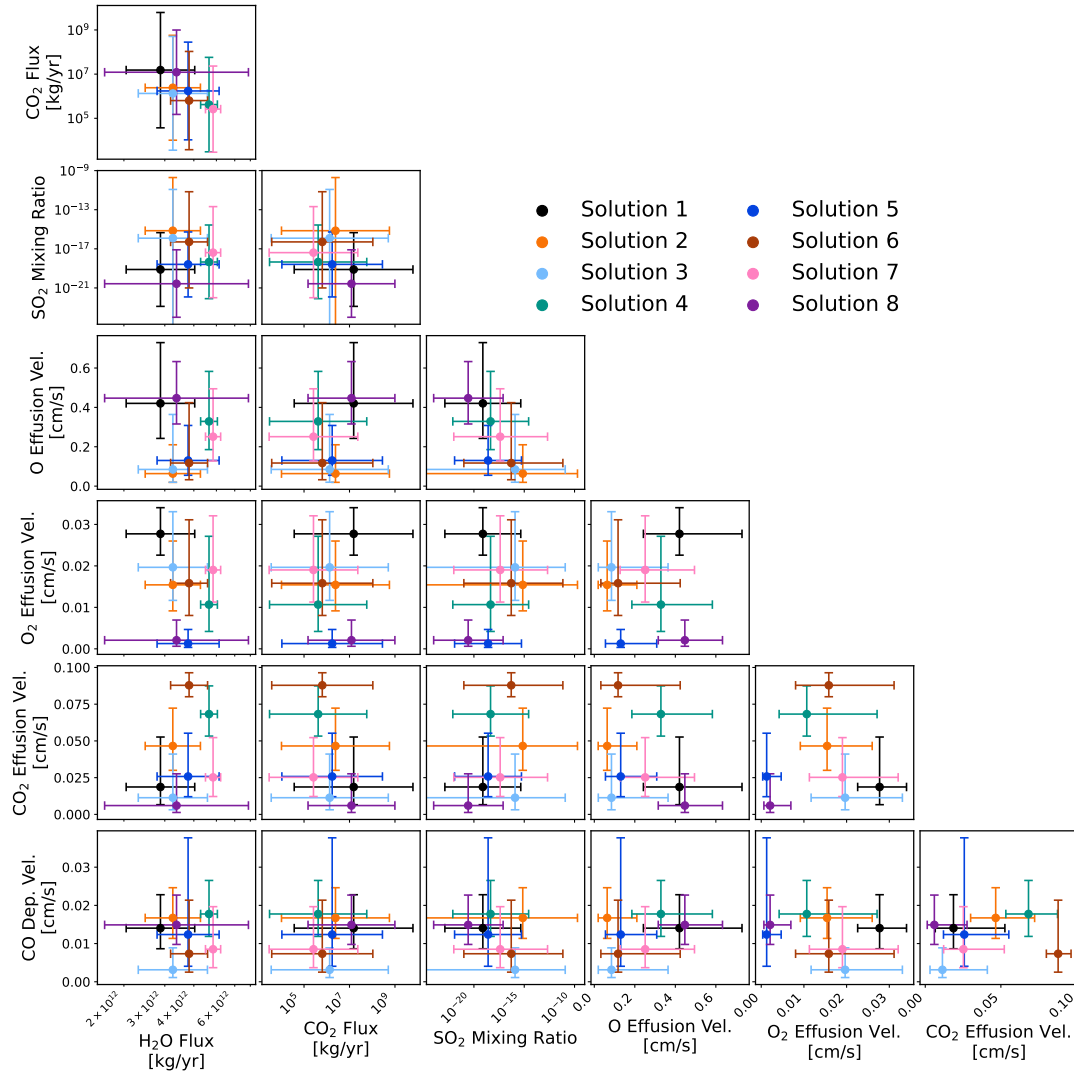


Figure 5.5: The relationship between all 8 solution means and 1σ error bars for all pairs of the 7 input parameters.

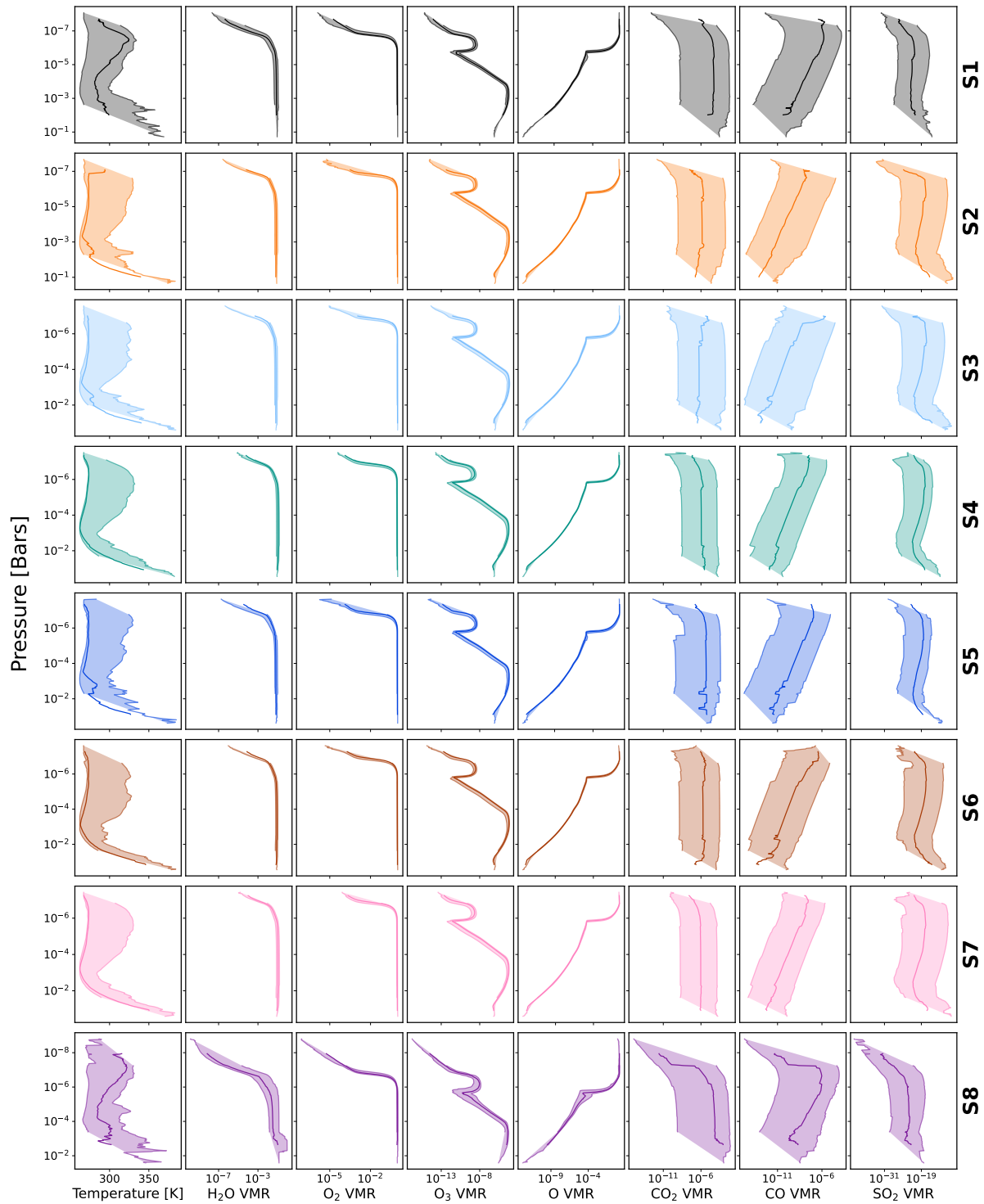


Figure 5.6: From left to right column, the pressure-temperature profiles and H₂O, O₂, O₃, O, CO₂, CO, and SO₂ volume mixing ratio profiles for all 8 solutions in the presented GMM constrained set; solutions 1 (S1) through 8 (S8) correspond to rows from top to bottom. The 50th percentile line and 1 σ shaded region are shown for every profile.

they contain significantly more data points than the MIRI photometric observations collected across two observing campaigns.

3.4 Constraints on Planetary Interior

If water and carbon dioxide outgassing rates are restricted to the maximum and minimum ranges from the 8 GMM solutions (shown in the left two columns of Figure 5.5), then considering the work of Thomas et al. (2025) would imply that T-1c is more likely to have an Earth-like magma emplacement rate with a wet mantle and CO₂-poor magmas. Figure 5.10 shows constraints on several of the baseline interior properties from Thomas et al. (2025) found when limiting the H₂O and CO₂ outgassing fluxes to the range found in this work. The interior property distributions significantly changed from their baselines were magma emplacement rate, mantle water content, and magma CO₂ content. The indicated interior parameters are consistent with Earth’s magma emplacement rate and mantle water content, and the implied CO₂ content is consistent with mid-ocean ridge basalts, which typically have m_{CO_2} less than 400 ppm wt% (Sigurdsson et al., 2015). Other parameters considered in Thomas et al. (2025) that are not included in Figure 5.10 do not change significantly from their baseline distributions, suggesting that the volatile content exerts the strongest influence on the outgassing rates when the mantle water fraction is this high. In this region of parameter space, T-1c is implied to have a H:C ratio in the source magma that is at least as high as Earth’s MORBs. Connecting this to the bulk mantle H:C ratio and to planetary formation could be the subject of future work.

4 Discussion

Using a disequilibrium photochemical model and realistic climate profiles (constrained by Gialluca et al., 2026, In Review) within a Bayesian inference framework, we have identified several solution sets of atmospheric boundary conditions which all indicate that thin (<0.5 bar) O₂-dominated atmospheres are the best atmospheric fit to the TRAPPIST-1c JWST emission data (Gillon et al., 2026; Zieba et al., 2023). Considering atmospheres supported by water and CO₂ outgassing only, the posterior favors high water outgassing, low CO₂ outgassing, and low atomic O top-of-atmosphere escape, while showing no strong preference for O₂ effusion, CO₂ effusion, or CO deposition velocities. Notably, every atmospheric solution shows ozone features, of which the 9.6 μ m emission band is the strongest. Our atmospheric solutions either possess extremely low pressures, at the millibar level, with higher CO₂ ($\sim$ 0.1 ppm) — or higher pressures ($\sim$ 0.1 bar) with low CO₂.

In section 4.1, we begin by discussion the preferences in input boundary conditions reflected by the inferred posteriors, as well as the resulting compositions and photochemical trends in our solution sets. Then we consider the spectra corresponding to our solutions in section 4.2, as well as potentially detectable features in future observing campaigns. Finally we cover the limitations of this study in section 4.4.

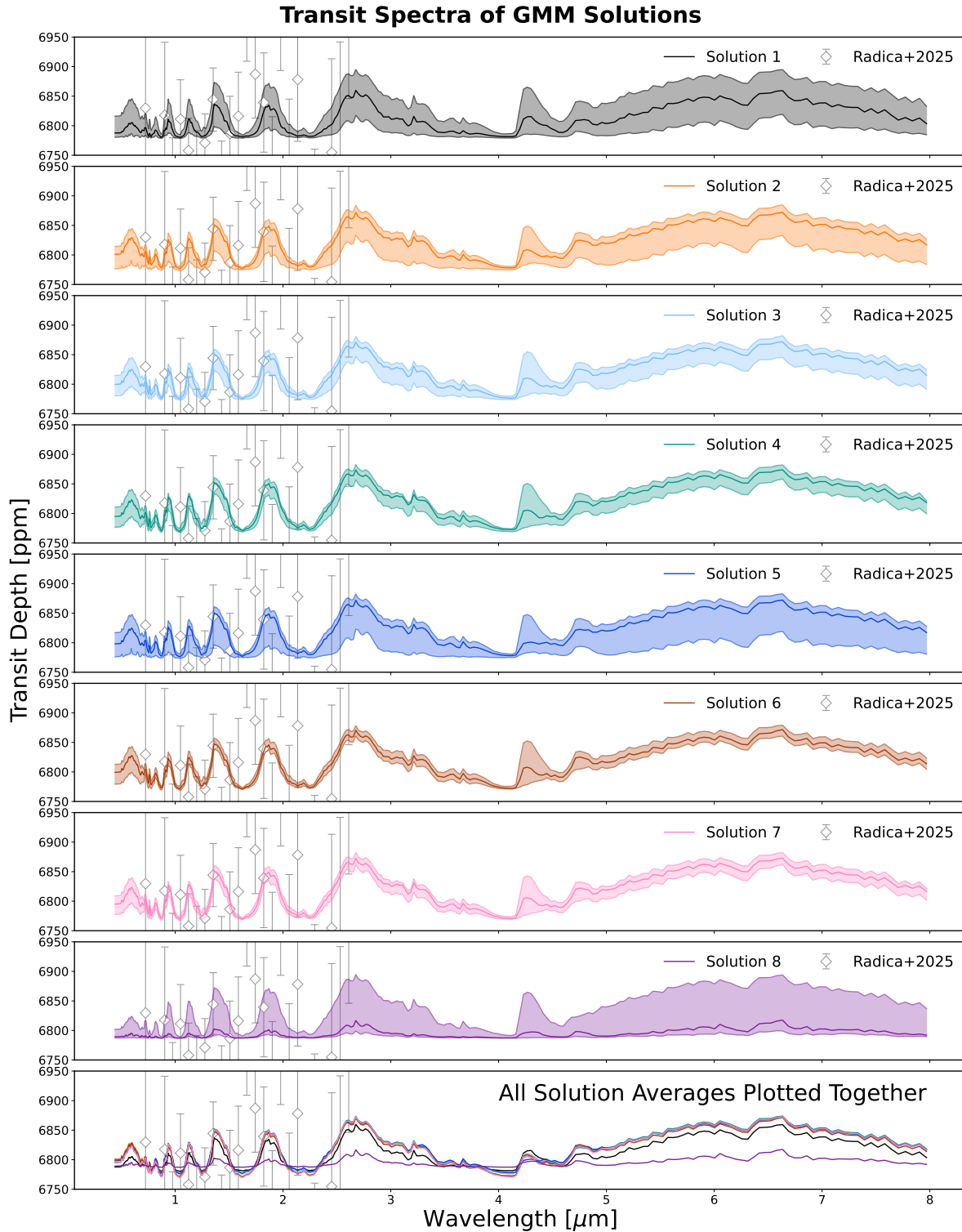


Figure 5.7: The 50th percentile and 1 σ region of transit spectra for each of the 8 GMM solutions (1 through 8 from top to bottom). The last row shows the solution median lines plotted together for easy comparison. T-1c JWST transmission data from Radica et al. (2025) is plotted for comparison.

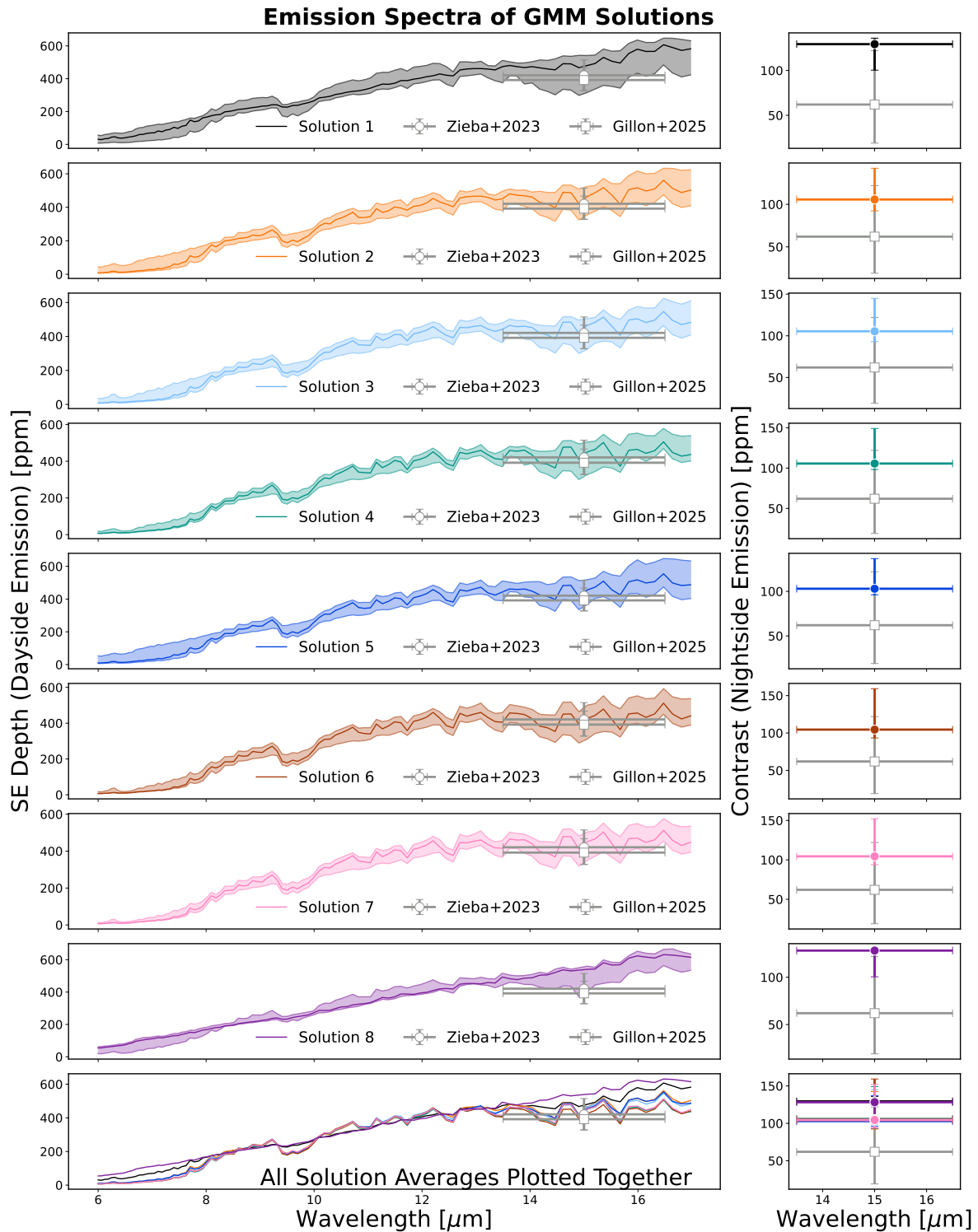


Figure 5.8: Same as Figure 5.7 except for the dayside emission spectra (left) and nightside $15\mu\text{m}$ emission (right). T-1c JWST emission data from Gillon et al. (2026); Zieba et al. (2023) is plotted for comparison.

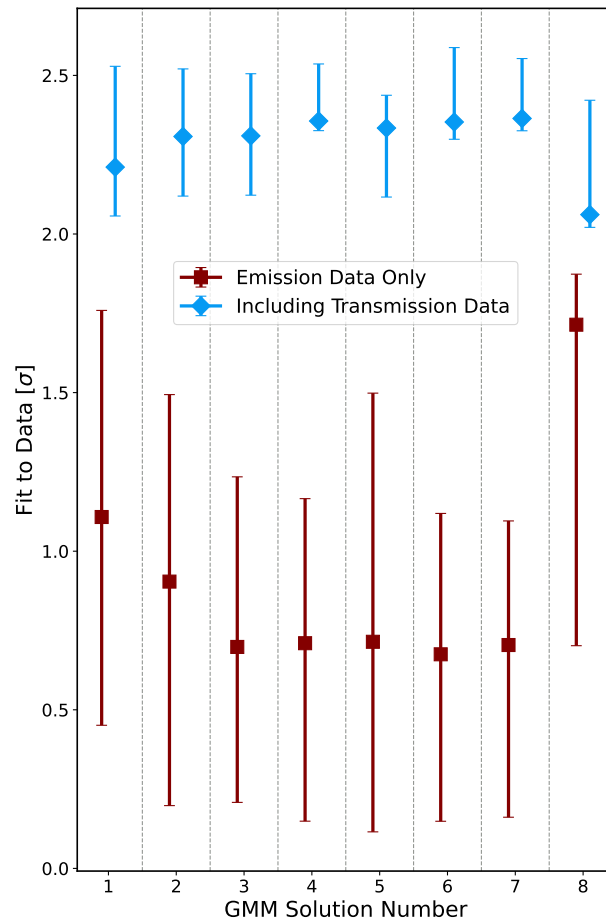


Figure 5.9: The σ fits of the 8 GMM solutions to the T-1c emission data only (Gillon et al., 2026; Zieba et al., 2023) (red points) and to the joint emission and transmission (Radica et al., 2025) data. Joint fits are more heavily weighted towards transmission, as there are more observational points in that dataset.

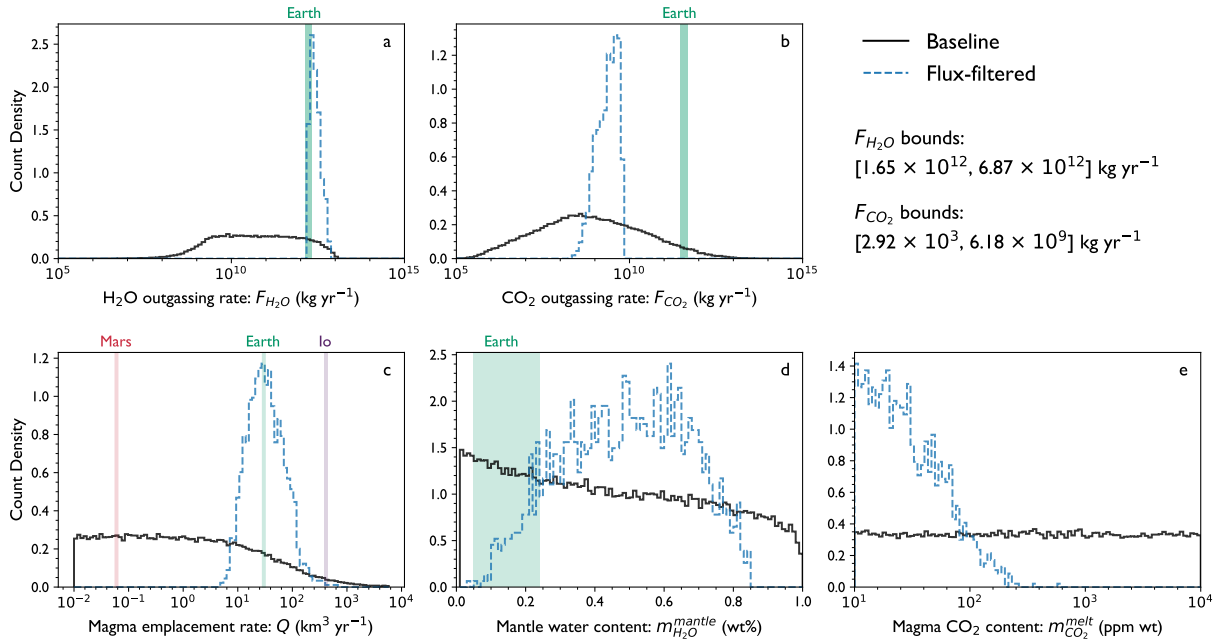


Figure 5.10: Posterior distributions for T-1c interior properties from [Thomas et al. \(2025\)](#) when H₂O and CO₂ outgassing fluxes are restricted to the ranges consistent with the 8 GMM Solutions. Top row: H₂O (left) and CO₂ (right) outgassing rates. Bottom row, from left to right: magma emplacement rate, mantle water content, and magma CO₂ content. The ‘flux-filtered’ distributions (dashed blue lines) are model runs from the baseline distribution of [Thomas et al. \(2025\)](#) (black lines) that result in H₂O and CO₂ outgassing rates within the bounds of the GMM solutions. Interior properties presented in [Thomas et al. \(2025\)](#) that were not significantly constrained by this work from their baselines are not shown.

4.1 Input Preferences & Atmospheric Compositions

When constraining the highest likelihood boundary conditions to generate atmospheres stable against collapse and matching the T-1c emission data with *MultiNest*, several preferences for input forward model parameters were identified including high H₂O flux and low CO₂ flux, SO₂ trace surface mixing ratio, and atomic O effusion velocity (see Figure 5.1). Conversely, the sink terms governing O₂, CO₂, and CO loss presented relatively flat posteriors (see Figure 5.1), indicating that the resulting atmospheres are not sensitive to these variables in the range of their priors. The preference for a low CO₂ outgassing flux is explained by the sensitivity of the 15 μ m bandpass to the presence of CO₂. In the current study, we only include the public T-1c emission data (Gillon et al., 2026; Zieba et al., 2023) in our likelihood calculation, which is all within the MIRI 15 μ m bandpass. The T-1c measurements at this wavelength are approximately 1.7σ below the expected dayside equilibrium temperature blackbody (Zieba et al., 2023), suggesting relatively low absorption from an atmosphere, or a surface composition with a higher bond albedo. Consequently, possible CO₂ outgassing in our models must be small to prevent build-up and significant 15 μ m absorption.

The preference for a higher H₂O outgassing flux is due to its role as the primary atmospheric source; atmospheric generation in our models is only possible through the release of H₂O or CO₂ and subsequent photochemistry, and as noted CO₂ is restricted to be low because of its influence on 15 μ m emission. Additionally, as we were focused on exploring the possible atmospheric solutions to the data, atmospheres that collapsed entirely were also rejected in this framework. Since there needed to be a high enough outgassing flux of material to prevent atmospheric collapse, and CO₂ is restricted to be low, a higher H₂O source flux was required for atmospheric generation.

Similarly to H₂O, the preference for a low atomic oxygen effusion velocity is likely to prevent atmospheric collapse. Across both the HL and GMM solution sets, atomic oxygen becomes the dominant species in the upper atmospheres, and ultimately the net loss flux of a species is a function of its effusion velocity and number density. Since the number density of O is highest at the top of the atmosphere (approaching a VMR of 1, see Figures 5.2 and 5.6), the loss is not supply limited. To prevent loss rates that are so high they lead to atmospheric collapse, the effusion velocity of O must be small. In contrast, the other species allowed to escape (O₂ and CO₂) become minor constituents at the top of the atmosphere; thus, they are supply limited, and even if the effusion velocity is large, their small number densities prevent problematic loss rates. Similarly, at the surface layer CO is a minor constituent, so there is no strong preference for deposition velocity because the supply limitation prevents a high net depositional flux.

Unlike other input dimensions discussed, the preference for low SO₂ trace mixing ratio is likely an artifact of the model’s inability to converge in high SO₂ regimes. Forward model calls with higher SO₂ fractions were unable to achieve the timestep convergence requirement (10^{17} s, or ~ 3 Gyrs), often only reaching lengths of $\sim 10^8$ s (or ~ 3 yrs). This was most commonly caused by instability in the H₂O mixing ratio leading to the generation of sulfuric acid; this scenario suggests sulfuric acid clouds would likely be created, but we limited this study to clear-sky atmospheres. An updated model properly accounting for cloud and haze formation may find these atmospheres in the high SO₂ region of our parameter space could be stable, but that was not considered in the current work. Thus, models rich in SO₂ were

rejected as unstable in the current framework. Additionally, although SO_2 is a greenhouse gas, the $15\mu\text{m}$ bandpass is much more sensitive to CO_2 than SO_2 at the low abundances tolerated here, and so the likelihood calculation is generally insensitive to the presence of trace SO_2 in the current study. In the future, if observations are considered that may be near wavelengths in which SO_2 is more influential than other radiatively active gases, it would be more prudent to properly account for sulfuric acid formation and explore high- SO_2 regions of the parameter space.

The models constrained by *MultiNest* presented in our solution sets are found to all be O_2 -dominated ($>85\%$ at the surface), with between $\sim 1 - 10\%$ H_2O (see Figures 5.2 and 5.6). Slight variations are seen in the atmospheric composition depending on how much CO_2 was possible. The biggest relationship that emerges in our results is that CO_2 varies inversely with atmospheric pressure. Overall the CO_2 in our solutions ranges from $\sim 0.001 - 1000$ ppm, which corresponds inversely to pressures between ~ 1 mbar $- 0.5$ bar. As a direct result of CO_2 , CO is also inversely related to surface pressure, varying between $10^{-10} - 0.1$ ppm at the surface, though it can get as high as a few ppm in the upper atmosphere. The reason for this carbon-pressure relationship is again tied to the strength of CO_2 absorption in the $15\mu\text{m}$ bandpass. If the surface pressure is low, the spectral continuum is high and closest to the planet’s equilibrium dayside temperature — in this case, the spectrum can tolerate more apparent absorption at $15\mu\text{m}$ from CO_2 and a small rise in nightside surface temperature, still match well to the MIRI measurements (Gillon et al., 2026; Zieba et al., 2023). Conversely, higher surface pressures lead to more heat redistribution and a lower spectral continuum which may already be in line with the measured $15\mu\text{m}$ emission, thus additional CO_2 would cause an apparent spectral feature that is too deep.

While the bottom of the atmosphere is dominated by O_2 and water, as altitude increases ozone also increases with O_2 and H_2O photolysis, reaching a peak of ~ 50 ppm near 0.1 mbar. In the uppermost atmosphere, photolysis of O_3 begins to produce atomic O more efficiently. Rapid destruction of H_2O and O_2 at $\sim 10^{-7}$ bar leads to a second local maximum of O_3 and additional O . By the top-most layer of the atmosphere, atomic O is the dominant constituent at $>>90\%$. The altitude profiles of CO_2 and CO remain relatively constant, though CO_2 begins to decrease in the upper atmosphere with increased photolysis and CO slowly increases from the surface, as production from CO_2 destruction increases, and it moves away from its surface deposition sink.

4.2 Spectra Solutions & Future Observational Discriminants

Spectral features seen in the atmospheres of this study are generated primarily by H_2O , CO_2 , and O_3 . All transmission and emission spectra from the GMM and HL solution sets match within 1σ uncertainty due to their consistent compositions (Figure 5.7 and 5.8). With the exception of solution 8 in the GMM set, every solution presented in the HL and GMM sets displays a clear $9.6\mu\text{m}$ ozone feature. This is in contrast to the results of Gialluca et al. (2026, In Review), which found that many O_2 -dominated atmospheres supported only by water outgassing (without any CO_2) were lacking in any ozone spectral features due to its rapid destruction by OH . Even in our higher pressure (~ 0.1 bar) CO_2 -poor atmospheres, there is a non-zero outgassing rate of CO_2 ; thus, we find that even a small amount of CO_2 , and subsequently produced CO , is sufficient to suppress OH and allow ozone to build up to

possibly detectable levels. Notably, this ozone feature at $9.6\mu\text{m}$ is present even when CO_2 is not clearly detectable at $15\mu\text{m}$ (e.g., Figures 5.3 and 5.8). The weaker ozone features in transmission, at 0.6 and $4.7\mu\text{m}$, are also typically present (Figures 5.3 and 5.7), though within the lower uncertainty on GMM solutions these appear to be less detectable than O_3 in emission. This result suggests that detection of O_3 in an atmosphere dominated by O_2 and water could be an indirect sign that CO_2 is being outgassed, suppressing ozone’s primary destruction pathway.

Lower emission depth at $15\mu\text{m}$ may either be caused by small amounts of heat redistribution in a thicker atmosphere, or by CO_2 absorption. The best way to break this degeneracy is to look for the $4.2\mu\text{m}$ CO_2 transmission feature in absorption, which is not present in thicker, CO_2 -poor atmospheres (e.g., Figure 5.3 shows both scenarios). Although it was reported as the least likely scenario, solution 8 in the GMM set has the lowest surface pressure, leading to very muted spectral features which are likely not detectable from a bare rock with current observing facilities.

Further observations would be needed to distinguish the atmospheric solutions in this study from best fit bare-rock scenarios. Overall, the atmospheres in this study compared to the dayside T-1c emission data (Zieba et al., 2023) provide slightly better matches ($\lesssim 1\sigma$) than the expected equilibrium dayside blackbody ($\sim 1.7\sigma$), but match equally as well as the best-fit ultramafic bare rock surface ($< 1\sigma$, Gillon et al., 2026). This is in agreement with the conclusions of Gillon et al. (2026), who considered the currently available emission data and independently concluded the planet likely either possesses no atmosphere or a tenuous oxygen atmosphere < 1 bar. Including transmission data (Radica et al., 2025), our atmospheres match equally as well as a flat line ($\gtrsim 2\sigma$). However, stellar contamination in transmission may still affect the current data (Radica et al., 2025), so future transit spectroscopy with novel contamination removal techniques (e.g., Allen et al., 2025; Rathcke et al., 2025) would be useful to improving T-1c interpretations. Given the clear ozone (at $9.6\mu\text{m}$) and water (shortward of $9\mu\text{m}$) absorption in emission, it would be useful to conduct further MIRI emission spectroscopy with LRS — giving the user the ability to bin the spectra to known feature sizes and locations — or MIRI photometry in the $10\mu\text{m}$ (for ozone) or $7.7\mu\text{m}$ (for H_2O) filters.

4.3 Astrobiological Importance of Constraining Atmospheric Fluxes

Through the current work, we have demonstrated the use of a photochemical model and a statistical framework to derive constraints from observational data on atmospheric outgassing and maintenance against escape processes. In this application, we consider a planet with a possible tenuous atmosphere, which would require constant balanced replenishment and loss in the harsh stellar environment of T-1. But, this same approach will be vital to contextualizing potential biosignature detections for more habitable planetary candidates. For a biosignature gas, isolating the production flux of that species allows you to begin connecting it to possible abiotic or biotic production processes. For example, methane production through Earth’s biosphere is one to two orders of magnitude greater than production through abiotic processes (e.g., serpentinization; Krissansen-Totton et al., 2018), yet methane is still a trace gas in our atmosphere. Connecting the small abundances of methane to its large surface flux through consideration of photochemical interactions with other species allows

us to identify it as a biosignature. This is one example of how flux-based inference models will be necessary to biosignature detection in the era of HWO.

4.4 Study Limitations

Across this study, several assumptions and approximations may have the potential to affect the interpretation of T-1c atmosphere models in the future. Firstly, due to the steep computational cost (driven by radiative transfer calculations), we replace self-consistent climate modeling in our forward model framework with a look-up database of pre-computed climate profiles from [Gialluca et al. \(2026, In Review\)](#). The use of a climate approximation can affect the computed atmospheric composition and spectra compared to a fully self-consistent model. However, due to the low surface pressures (<0.5 bar) and lack of prevalent greenhouse gases in the atmospheres in this study, the globally averaged surface temperature of every case remains (and is expected to be) close to T-1c’s equilibrium temperature of 340 K; thus, we don’t anticipate that self-consistent climate calculations will significantly change our resulting thin atmospheres. Furthermore, in some cases across the GMM solutions, specific forward models comprising the solution cluster would select differing pressure-temperature structures in the upper atmosphere (reflected by the regions of uncertainty shown in Figure 5.6), yet these differences did not significantly affect the resulting bulk atmospheric composition or spectra. Finally note, the solely O_2 -dominated atmospheres found in this study are a subset of the compositions explored in [Gialluca et al. \(2026, In Review\)](#), who found very minor variations in climate profiles when the bulk atmosphere remained the same, again suggesting that self-consistent climate calculations would not significantly affect the results of the current study. In the future however, if this method is applied to other planets expected to have very thick atmospheres or those rich in greenhouse gases (especially condensible species, like water), the absence of self-consistent climate calculations could have a much larger influence on results. We would caution future work to carefully assess the suitability of the climate solution used for a given target.

While it is not a limitation that affects the accuracy of results in this work, we would also like to note that the modeling framework used here required high computational expense. That is, our results necessitate several months of runtime on a 192 core super computing node. This computational cost is due in large part to radiative transfer calculations, which is also the reason why self-consistent climate modeling is too costly to include in the framework. Future work may explore additional fast climate or radiative transfer methods to make a study like this more feasible for additional planetary targets or for research groups that have access to limited high performance computing clusters.

In this work, we limited outgassing to H_2O and CO_2 , but a more diverse outgassing source with additional species could change the possible atmospheric solutions. Methane in particular was not included as an outgassed species, but is known to be a minor outgassed species on the Solar System terrestrials (e.g., [Gillmann et al., 2022](#); [Gold, 1982](#); [Yung et al., 2018](#)), and it is even the primary atmospheric constituent of the rocky moon Titan (e.g., [Lunine & Atreya, 2008](#)). The methane outgassing rates for T-1c constrained by ([Thomas et al., 2025](#)) span to negligible values, supporting the validity of the atmospheric scenarios presented here; however, higher methane outgassing remains possible and represents a valuable avenue for future work. Similarly, while we considered very trace amounts of SO_2 , most models that

tested SO_2 at percent levels were unstable due to the likely formation of sulfuric acid clouds, which were beyond the scope of this study. Given the Solar System examples of an SO_2 dominated atmosphere on Io (Lellouch, 2005) and sulfur chemistry with cloud formation on Venus (Krasnopolsky, 2015), future work could consider SO_2 as the bulk outgassed species, with or without the presence of water to facilitate cloud formation.

Clouds, hazes, and dust also have the potential to affect the type of atmospheres we could observe for the TRAPPIST-1 planets. Often aerosols can complicate climate and photochemical processes in the atmosphere, leading to increased computational expense that was not affordable in this study; we chose to focus this novel method on the generation of clear-sky atmospheres. Furthermore, Earth-like water clouds on T-1c are unlikely in the pressure-temperature regime we consider (Helling, 2019), additionally there was no reported water condensation in our simulations. Water clouds have the potential to play a larger role for the outer planets in the TRAPPIST-1 system (as discussed in Gialluca et al., 2026, In Review). As previously noted, increasing SO_2 at the surface generally indicated the likely formation of sulfuric acid clouds, which we did not explore in this work. If sulfuric acid clouds are present on T-1c, it may mute transmission spectral features, though emission should be more robust against this effect (Lustig-Yaeger et al., 2019a). Dust and hazes may have a more pronounced effect on T-1c atmospheric scenarios, especially considering the low pressures of our modeled cases. It is known that dust on Mars can represent a temporally varying source of spectral confusion, potentially increasing the emissivity of the $15\mu\text{m}$ CO_2 band (Kahre et al., 2017). Dust may also significantly increase reflectivity (Gao et al., 2021), making it an important consideration for the future Habitable Worlds Observatory. Organic haze formation has also been suggested to be more efficient in M dwarf planetary atmospheres (Arney et al., 2018, 2016), though this is most often in atmospheres with methane present, which we did not consider here. Future studies could improve on this work by considering the affect of different aerosols on the atmospheric spectra and climate profiles of our atmospheres.

5 Conclusions

In this study we have used Bayesian nested sampling (via *MultiNest* Buchner et al., 2014; Feroz et al., 2009) to determine the set of boundary source and sink parameters that generate atmospheres which best match the current TRAPPIST-1c emission data (Gillon et al., 2026; Zieba et al., 2023) when considering atmospheres generated solely by plausible water and CO_2 outgassing (Thomas et al., 2025). Our forward model includes a photochemical model (Arney et al., 2016; Gialluca et al., 2026, In Review; Kasting et al., 1979; Meadows et al., 2018a) and a climate profile selection scheme based off the stable atmospheres of Gialluca et al. (2026, In Review). For every possible set of inputs identified as likely solutions by the inference framework, we find that the resulting atmosphere is thin, ~ 1 mbar – 0.5 bar, O_2 -dominated, with between 1 – 10% water at the surface level. Because the T-1c emission data is constrained to the $15\mu\text{m}$ bandpass which is extremely sensitive to the presence of CO_2 , the CO_2 abundance of these solutions vary inversely with atmospheric pressure, always maintaining a shallow emission consistent with the measurements of Gillon et al. (2026); Zieba et al. (2023). Overall, the CO_2 abundance at the surface level reaches ~ 0.1 ppm at maximum. The high H_2O and low CO_2 outgassing rates preferred in the posteriors

suggest an Earth-like magma emplacement rate, high mantle water content, and low magma CO₂ content (Thomas et al., 2025). Across all solutions, spectral features from H₂O, CO₂, and O₃ (particularly in the 9.6 μ m emission band) may be observable in the future. This work suggests thin outgassed O₂ atmospheres may be easily generated and maintained on TRAPPIST-1c.

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CHAPTER 6

DISCUSSION

Ancora imparo

– Michealangelo

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Coinciding with the launch of JWST, the first telescope with the capability to probe high mean molecular weight terrestrial exoplanet atmospheres, the work contained in this dissertation is one of the earliest comprehensive studies of exoplanet environmental characterization. Through this body of work, we have demonstrated that M dwarf planets can generate and maintain tenuous secondary outgassed atmospheres, and that these types of thin atmospheres are still consistent with JWST observations for the TRAPPIST-1 system.

Here we discuss the novel work completed in this dissertation which represents a holistic approach to exoplanet atmospheric characterization, taking into account extensive available observational and theoretical context on a particular planetary system (§1). In particular, we consider the evolution of likely star-planet radiative interactions, atmospheric processes (photochemistry, climate, radiative transfer, escape), plausible geochemical outgassing, and all available JWST observations of the TRAPPIST-1 system to best characterize the potential planetary atmospheres. Furthermore, we discuss the ways in which this thesis supports astrobiological searches now and in the future (§2), including defining biosignature false positive scenarios and outlining how comparative planetology can be used to learn about habitable zone planets from observations of their hotter interior neighbors. Finally, we consider avenues of ongoing and future work at the cutting edge of the field (§4).

1 A Holistic Approach to Characterizing Terrestrial Exoplanets

Across this body of work, we have provided a detailed case study demonstrating the use of multiple modeling techniques to understand the terrestrial exoplanet system TRAPPIST-1, and maximize information from a limited dataset by leveraging the known physics and chemistry dictating atmospheric processes and star-planet interactions. This comprehensive modeling approach has allowed us to unequivocally show that it is possible to generate and maintain tenuous secondary atmospheres through plausible geochemical outgassing for irradiated M dwarf planets (like those in the TRAPPIST-1 system), despite their high expected atmospheric escape rates (e.g., [Dong et al., 2018](#)).

Before the advent of JWST’s sensitive TRAPPIST-1 observing campaigns, we use limited prior information on TRAPPIST-1 to begin constructing possible evolutionary pathways of the planets, including knowledge of stellar evolution, planetary separation from the host, and early HST observations confirming the lack of an H₂-dominated primary atmosphere ([De Wit et al., 2018](#); [Wakeford et al., 2019](#)). Specifically, we model the loss of water over time caused by thermal hydrodynamic atmospheric escape on the TRAPPIST-1 planets driven by the XUV evolution of the host star from formation through the present. Through this type of precursor work, observational discriminants can be identified that form the foundation for observing justifications with more comprehensive missions, like JWST. In the case of TRAPPIST-1, species like CO₂ and O₂ were quickly recognized as key secondary atmosphere constituents in line with the expected stellar-driven evolution (e.g., [Gillon et al., 2020](#); [Meadows, 2017](#)). In a similar vein, we use this foundational system knowledge to model the evolution of volatiles on the TRAPPIST-1 planets ([Gialluca et al., 2024](#)) (§3), providing fundamental information on maximum energy- and diffusion-limited hydrogen escape rates,

water loss over time, and oxygen generation following water photolysis. Constructing this basis of information is key to informing selected physical processes to include in later work. For example, [Thomas et al. \(2025\)](#) used our constraints on maximum hydrogen escape rates ([Gialluca et al., 2024](#)) to bound the possible water outgassing rates in the system, ensuring that the assumed outgassing did not produce an H_2 -dominated atmosphere at present-day (consistent with transmission observations of the system, [De Wit et al., 2018](#)).

The planetary and volatile evolution foundational knowledge of our first project, combined with the collaborative study on outgassing in the system ([Thomas et al., 2025](#)), then allowed us to build to self-consistently modeling the generation and maintenance of outgassed secondary atmospheres. The first project in this body of work provided an informed atmospheric starting point for present-day models to evolve from: thin (0.1 bar) dry O_2 -dominated, consistent with other analyses in the community (e.g., [Lincowski et al., 2023](#); [Zieba et al., 2023](#)). Additionally, [Thomas et al. \(2025\)](#) provided the atmospheric source boundary condition, while further collaboration with aeronomy experts informed possible oxygen and carbon escape rates. With this background work, the second project in this thesis arc modeled the generation of outgassed atmospheres, identifying a range of compositional archetypes that could arise in the plausible phase space of boundary conditions including oxygen, steam, and carbon-bearing bulk compositions. Coinciding with the onset of observational data on the TRAPPIST-1 planets ([Allen et al., 2025](#); [Ducrot et al., 2025](#); [Espinoza et al., 2025](#); [Gillon et al., 2026](#); [Glidden et al., 2025](#); [Greene et al., 2023](#); [Lim et al., 2023](#); [Piaulet-Ghorayeb et al., 2025](#); [Radica et al., 2025](#); [Zieba et al., 2023](#)), our second study provided comprehensive grid sweeps of atmospheric solutions that still fit well to JWST data on the planets, informing future observational discriminants of interest. This study benefited from full self-consistency resulting in photochemical compositions that respond to changing sink processes and temperature structures. Consequently, we built up a library of unique atmospheric solutions and temperature profiles, which enabled the final project of this thesis.

Transitioning to the final project of this thesis, the intuition and models developed in prior chapters describe what is *possible* for the TRAPPIST-1 planetary atmospheres, allowing us to move into a more statistical framework to ask what is *likely*. Prior to the grid sweep studies of Chapter 4, we had no prior knowledge of 1) what plausible outgassed atmospheres could look like or how broad the compositional phase space would be; 2) the degree to which climate profiles could differ and what factors most strongly influenced them; or 3) which boundary conditions would meaningfully affect the resulting atmospheric profiles. The grid sweeps (Chapter 4) addressed each of these unknowns, allowing us to construct a Bayesian inference pipeline with well-motivated input parameters, defined flat prior ranges known to span stable solutions, and most importantly we were able to implement a fast approximate climate profile selection scheme that circumvented the need for expensive climate model runs during inference. Ultimately, we were able to identify the most likely atmospheric solution (thin O_2 -dominated) for TRAPPIST-1c when fitting the current emission data ([Gillon et al., 2026](#); [Zieba et al., 2023](#)), and further we explored the observational discriminants of this solution and what it means for the likely geochemical properties of the planet.

Across this thesis, we have maximized the information content of one of the first exoplanetary systems to have atmospheric observations sensitive enough to probe high mean molecular weight secondary atmospheres. We have leveraged a variety of approaches including evolutionary modeling of star-planet interactions, self-consistent photochemical-climate

modeling, interdisciplinary collaboration, and Bayesian inference in retrieval-like frameworks. By completing the three studies in this body of work sequentially, we have provided one of the most in depth analyses on the characterization of atmospheres for Earth-sized terrestrial planets to date. We have shown that thin atmospheres can be generated and maintained through geochemical outgassing against the harsh stellar environment of an M dwarf star. Altogether, these projects analyze a planetary system considering all available information on the context of its environment, as opposed to considering evolutionary processes or observed spectral features in isolation.

2 Astrobiological Implications of this Work

In this thesis we have placed a particular focus on considering a planet’s environmental context when conducting characterization, in line with the biosignature standards of evidence outlined for the community when assessing the potential for life on another planet (Meadows et al., 2022). Although there is currently no clear identification of potential biosignatures on the TRAPPIST-1 planets, the standards of evidence framework still provides a useful outline for how to best characterize exoplanet atmospheres, and following it prepares us for any possible biosignature detections that may arise in the future. Furthermore, the most robust TRAPPIST-1 observations at this point have been emission observations of the interior planets, as transmission studies are prone to extreme stellar contamination (e.g., Howard et al., 2023; Lim et al., 2023; Rathcke et al., 2025); thus, little is known about the atmospheres of the habitable zone planets. Consequently, one of the best sources of information on the potentially habitable planets is through comparative planetology with their better-observed interior neighbors. Considering the five-question framework of Meadows et al. (2022), the work in this thesis may contribute to addressing questions 1 through 3 (have you detected and adequately identified a signal, and are there abiotic sources for your detection), supporting biosignature evaluation in the TRAPPIST-1 system should a candidate signal be identified in the future, as well as M dwarf systems in general.

The first level of the evidence framework, concerned with the detection and correct attribution of an authentic signal (Meadows et al., 2022), is directly related to the stellar contamination issues that have been plaguing transmission observations of the system. In the case of TRAPPIST-1c transmission data (Radica et al., 2025), most solutions, including a flat line, fail to fit the data to better than 2σ . However, using a novel approach calculating the Pearson Correlation Coefficient (PCC) (§3.3), we show a negative correlation between atmospheres with H₂O features and the transmission data, which appears to be unusually strong considering the size of errorbars on the datapoints. This PCC analysis indicates that there may be over-subtracted water features assumed to be in the M dwarf stellar atmosphere, potentially constituting an artifact in the dataset from pre-processing steps. This is particularly important in the context of biosignature standards of evidence because the presence or lack of water on TRAPPIST-1c can inform the likelihood of water on the habitable zone planets, providing extremely useful environmental context. In a separate example, the transmission data of the habitable zone planet TRAPPIST-1e has indicated the potential presence of methane or CO (Allen et al., 2025). By identifying strong absorption near $4\mu\text{m}$ in stable atmospheres containing even trace SO₂, we have shown that there could be

a potential source of confusion for the attribution of potential TRAPPIST-1e transmission signals near $4\mu\text{m}$ to methane, which is important because methane is a potential biosignature gas of interest. Other important contextual molecules for biosignature characterization that cannot be ruled out for TRAPPIST-1e at this time, namely oxygen and CO, have been extensively studied in this thesis, which brings us to question 3 of the biosignature standards of evidence.

This body of work provides extensive context for signs of outgassed atmospheres useful for addressing the third question of the evidence framework, concerned with identifying possible abiotic sources for a signal (Meadows et al., 2022). In particular, we have broadly considered the photolytic destruction of water as a production pathway for abiotic O_2 and shown that it can become the bulk constituent of a secondary atmosphere formed through either the loss of an initial surface volatile inventory or through steady water outgassing over time. Notably, these high O_2 atmospheres were found to be the best fit atmospheric solution for the interior planets, particularly TRAPPIST-1c (Chapters 4 and 5). In some cases, we have also shown that abiotic CO can build up and dominate the planetary atmosphere; notably, this occurs in the case of TRAPPIST-1e, which may still be consistent with current transmission data (Allen et al., 2025). Furthermore, in §3.4 we have shown quantitatively that these CO-dominated atmospheres can constitute a chemical disequilibrium false positive biosignature, originally theorized by Krissansen-Totton et al. (2016). Through this thesis, we have provided a robust demonstration that the potential biosignature species O_2 and CO may be expected common false positives in the M dwarf environment. This is important evidence for use when evaluating question 3 in the biosignature standards of evidence framework for similar planets in the future (Meadows et al., 2022).

Finally, through the use of coupled photochemical-climate simulations in Chapter 4, we were able to constrain the pressure-temperature profiles of tenuous TRAPPIST-1 planet atmospheric models in the context of the phase diagram of water. This allowed us to demonstrate that TRAPPIST-1d and e, which straddle the potential habitable zone (e.g., Kopparapu et al., 2013), may possess several tenuous atmospheres that lead to temperature regimes favorable for liquid water. Furthermore, we found that many hemispherically-average night-side temperature profiles for the interior planets TRAPPIST-1b and c are solidly within the liquid region of water’s phase diagram (§3.1.2). This suggests that even tenuous (<0.1 bar) atmospheres could produce traditionally habitable environments on the first 4 planets of the TRAPPIST-1 system. This work helps to expand our perspective on where habitable environments may arise, and suggests that future work should consider the potential for habitability on the nightsides of hot terrestrials.

3 Novel & Innovative Approaches of this Work

This thesis presents pioneering work for coupled photochemical-climate modeling that also considers the equilibration of atmospheric pressure and composition caused by balancing outgassing and atmospheric escape rates. This provides foundational knowledge for the community into how tenuous secondary atmospheres are outgassed and maintained, particularly on M dwarf planets which are subjected to intense stellar radiation (e.g., Baraffe et al., 2015; Ribas et al., 2005). Furthermore, accounting for this broad range of planetary processes and

their interactions required an extremely interdisciplinary and collaborative approach, including insights from astronomy, atmospheric science, geochemistry, and aeronomy. Moreover, we have presented one of the first studies to include a disequilibrium photochemical model in a retrieval-style statistical inference framework targeting constraints on atmospheric source and sink fluxes directly, instead of just total abundance. This approach is necessary for biosignature detection because the presence of a particular gas is not itself the biosignature; rather, it is the biospheric source flux of that gas that indicates biological production (Meadows et al., 2018b). The work to connect observational data to atmospheric source fluxes in this thesis represent novel pioneering steps towards full flux-based retrieval pipelines, necessary for NASA’s upcoming biosignature detection missions like the Habitable Worlds Observatory (National Academies of Sciences, Engineering, and Medicine et al., 2021).

4 Ongoing & Future Work

There are ongoing challenges in both interpreting the data of TRAPPIST-1 specifically, and in improving the community modeling suites for better atmospheric characterization in general. Here we discuss ongoing challenges facing the characterization of the TRAPPIST-1 system (§4.1), as well as future avenues for model development related to the atmospheric characterization of terrestrial exoplanets in general (§4.2).

4.1 Characterization of the TRAPPIST-1 System

Considering the TRAPPIST-1 data, one of the biggest unsolved mysteries at present is the contrasting emission behavior of TRAPPIST-1b in the $15\mu\text{m}$ and $12.8\mu\text{m}$ bandpasses (Ducrot et al., 2025; Greene et al., 2023). The $15\mu\text{m}$ measurement showed a brightness temperature close to the planet’s expected dayside equilibrium temperature, implying little to no heat redistribution or absorption (Greene et al., 2023). Thus, a subsequent $12.8\mu\text{m}$ observation would naturally be expected to fall on or above the dayside blackbody curve — either confirming the absence of an atmosphere or suggesting that the true continuum is hotter and the $15\mu\text{m}$ datapoint sits at the bottom of a CO_2 absorption feature. Instead, the $12.8\mu\text{m}$ observation revealed a measurement well *below* the expected blackbody curve (Ducrot et al., 2025). Since $15\mu\text{m}$ is a strong CO_2 absorption window while $12.8\mu\text{m}$ lacks strong absorbers, lower emission at $12.8\mu\text{m}$ suggests the $15\mu\text{m}$ feature may be in emission rather than absorption, potentially indicative of a strong atmospheric temperature inversion or an unusual bare rock composition. Photochemical haze has been invoked as a potential explanation (Ducrot et al., 2025), but detailed climate models do not currently support a haze-driven temperature inversion seen at $15\mu\text{m}$ in a CO_2 -rich atmosphere (Gillon et al., 2026). The TRAPPIST-1b data therefore remain unexplained by self-consistent modeling, representing a compelling open question for atmospheric characterization efforts.

Another active area of research for the characterization of TRAPPIST-1 and other M dwarf systems revolves around successful transmission observations of habitable zone and colder planets, which hinges on our ability to treat ongoing stellar contamination issues. Recent efforts have focused on observing the transit of an assumed-airless TRAPPIST-1b in succession with the planet of interest, allowing one to correct the transit spectrum using

variations seen in the airless planet’s observations (Allen et al., 2025; de Wit et al., 2023; Rathcke et al., 2025). However, this technique hinges on the presence of an airless planet and back-to-back transit windows, and TRAPPIST-1b is still not fully understood, as discussed in the context of the $12.8\mu\text{m}$ data above (Ducrot et al., 2025; Greene et al., 2023). A useful avenue of study may be to analyze broad spectra of M dwarf stars, with a particular focus on the temporally-varying stellar inhomogeneities and flaring events, to assist in the creation of better stellar contamination removal protocols.

4.2 Beneficial Model Developments for Exoplanet Characterization

Given the limited observational datasets available for terrestrial exoplanets, computational modeling is a vital tool that allows us to use our knowledge of physical principles (e.g., thermodynamics, chemistry, radiative transport) to bridge the gaps in our data, and suggest effective future observational discriminants. Accordingly, the self-consistency of modeling pipelines is crucial to ensuring the complex interactions between factions of the physical system (e.g., planetary interior, surface-atmosphere boundary, climate response) is properly accounted for. In this thesis, we have provided pioneering work into the construction of a full flux-based retrieval framework, aimed at constraining the atmospheric source fluxes as opposed to only focusing on gas abundance. However, we were unable to do this with a coupled climate model, which is necessary to correctly retrieving source and sink fluxes. For example, the common practice of assuming an isothermal profile in atmospheric retrieval can lead to order of magnitude differences in derived gas abundances (Barstow & Heng, 2020; Rocchetto et al., 2016). To truly constrain atmospheric maintenance fluxes, retrieval-like statistical inference pipelines will need to employ coupled photochemical-climate algorithms as their forward models; however, this is currently not possible due to the extreme computational expense of climate and isolated retrieval models. The large computational cost is primarily caused by radiative transfer calculations, which govern the absorption, emission, and scattering of radiation as a function of altitude, dictating heating and cooling rates and connecting atmospheric composition to observed spectra (Wendisch & Yang, 2012). A useful future avenue of research is to improve the computational efficiency of radiative transfer algorithms, while maintaining accuracy necessary for climate modeling and spectra generation. This challenge is already being considered as a target of machine learning by recent work (Malsky et al., 2025).

Another interesting area of work that is not well understood is the inclusion of non-local thermodynamic equilibrium (NLTE) processes in atmospheric modeling suites. An atmosphere is said to be in local thermodynamic equilibrium (LTE) when collisions between particles are frequent enough that their energy level populations are defined by the kinetic energy of the gas, described by Maxwell’s distribution (López-Puertas & Taylor, 2001). However, in very low pressure environments, collisions become infrequent, and the kinetic, vibrational, and rotational temperatures of a gas particle are no longer guaranteed to be equal, indicating the environment is in NLTE (López-Puertas & Taylor, 2001). This occurs at some high altitude in nearly every planetary atmosphere (including Earth Dickinson et al., 1987), and it may be especially relevant for planets that are found to potentially have very tenuous atmospheres, such as TRAPPIST-1b and c. NLTE effects can alter the heating and cooling rates of an atmosphere (Kutepov & Feofilov, 2024; López-Puertas & Taylor, 2001) and it

can cause unexpected behavior when comparing gas spectral features that are a product of different vibrational-rotational states (Wright et al., 2022). Due to these influences, NLTE effects can modify the physical states of an atmosphere and the information we retrieve from observations. Future work should consider how the inclusion of NLTE affects the results of planetary modeling pipelines.

CHAPTER 7

CONCLUSIONS

End? No, the journey does not end here

– JRR Tolkien, “*The Lord of the Rings*”

In this dissertation, we have provided an extensive characterization of the TRAPPIST-1 planetary system, considering their expected stellar-driven evolution, photochemistry, climate, outgassing, and atmospheric escape, guided by the earliest JWST observing campaigns. We began by using knowledge of M dwarf XUV evolution to model the volatile loss history of the TRAPPIST-1 planets from formation to present-day, assuming an initial surface water inventory. Through this work, we showed that the planets are likely to generate massive amounts of abiotic O_2 through water photolysis, and furthermore that detection of oxygen on the interior planets may imply likely water retention on the habitable zone planets today. From there, we took this informed high- O_2 starting point, along with plausible outgassing rates for the planets, and applied a novel method to generate comprehensive grids of coupled photochemical-climate models that also allow surface pressure equilibration due to the balance of outgassing, escape, and photochemical interactions. Importantly, this allowed us to show that tenuous atmospheres can be supported by outgassing and maintained against strong stellar-driven atmospheric escape for the TRAPPIST-1 planets. We identified 6 different atmospheric compositions, arising naturally from water and CO_2 outgassing, that may still be consistent with all emission and transmission data taken in the system. Finally, we transitioned to a statistical approach, pioneering one of the earliest examples of employing a coupled photochemical-radiative transfer pipeline as the forward model for an atmospheric retrieval-like statistical inference framework. This method allowed us to constrain the atmospheric boundary conditions directly as opposed to just targeting gas abundances. We applied this framework to TRAPPIST-1c, identifying several input sets of sources and sinks that matched the emission data to high likelihood, which all ultimately produced thin (1 mbar – 0.5 bar) O_2 -dominated atmospheres.

The projects in this thesis act as parts of a whole, demonstrating the characterization of an exoplanetary system using all available data and environmental context. The first project provided the foundational initial states to evolve present-day atmospheres from. The

second project built on this, using sophisticated physical models to generate self-consistent atmospheric and climate profiles that may exist on the planets today. Finally, the last project used these precomputed climate profiles to run a statistical population of models, moving from what is a possible atmosphere to what is a likely atmosphere for TRAPPIST-1c, based on its JWST observations. This approach has demonstrated how to maximize science return from limited spectroscopic datasets, and provides valuable information for future M dwarf biosignature searches, identifying alien atmospheres that may still be generated through abiotic processes. The current and next generation of NASA observing missions promise to usher in a new era of understanding for both planetary atmospheres and the search for life in the universe, they require our dedication to model improvement to continue advancing our understanding of these alien worlds.

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APPENDIX A

CURRENT CURRICULUM VITAE

Megan T. Gialluca

Curriculum Vitae; ORCID: 0000-0002-2587-0841
NSF Graduate Research Fellow & PhD Candidate
Astronomy & Astrobiology, University of Washington

Education

University of Washington

Dual Title PhD in Astronomy & Astrobiology
M.Sc. in Astronomy
Graduate Coursework Cumulative GPA: 3.89

Sept 2021 – June 2026
Sept 2021 – March 2023

Northern Arizona University

B.Sc. in Astronomy & Physics; Summa cum laude
Cumulative GPA: 3.96, Major GPA: 4.0

Sept 2017 – April 2021

Relevant Work Experience

- **Graduate Research Assistant**; University of Washington. June 2022 – Present
Advisor: Prof. Victoria Meadows.
- **PhD Intern**; Northrop Grumman & NASA Goddard Space Flight Center June 2024 – Sept 2024
NASA GSFC Advisor: Dr. Chris Stark. Northrop Advisor: Dr. Jon Arenberg.
- **Graduate Teaching Assistant**; University of Washington. Sept 2021 – June 2022
- **Research Assistant**; Lowell Observatory. May 2020 – Sept 2021
Advisor: Dr. Nick Moskovitz. NSF Funded Project Award no. AST-194482
- **Harvard CFA REU Internship**; Harvard Center for Astrophysics (CFA). June 2020 – Aug 2020
Advisor: Dr. Ana Bonaca. NSF Grant no. AST-185226
- **Public Programs Educator**; Lowell Observatory. Oct 2018 – May 2020

First Author Publications

- **Gialluca, M.T.**, Arenberg, J.W., Stark, C., et al., *Shedding Light on Large Space-Based Telescopes: Modeling Stray Light due to Primary Mirror Damage from Micrometeoroid Impacts*. *J. Astron. Telesc. Instrum. Syst.* 12(4), 041002 (2026) [[ArXiv Link Here](#); [SPIE Link Here](#)].
- **Gialluca, M.T.**, Barnes, R., Meadows, V.S., et al., *The Implications of Thermal Hydrodynamic Atmospheric Escape on the TRAPPIST-1 Planets*. *PSJ*, 5, 137. (2024)
- **Gialluca, M.T.**, Robinson, T.D., Rugheimer, S., and Wunderlich, F., *Characterizing Atmospheres of Transiting Earth-like Exoplanets Orbiting M Dwarfs with James Webb Space Telescope*. *PASP*, 133, 054401. (2021)
- **Gialluca, M.T.**, Naidu, R.P., and Bonaca, A., *Velocity Dispersion of the GD-1 Stellar Stream*. *ApJL*, 911, L32. (2021)
- **Gialluca, M.T.**, Meadows, V.S., Lincowski, A.P., et al., *A Self-Consistent Exploration of Plausible Atmospheres in the TRAPPIST-1 System from Theory and Observation*. [In Review at PSJ] (2026) [PDF Available on Request]
- **Gialluca, M.T.**, Meadows, V.S., Lincowski, A.P., et al., *Matching Atmospheric Boundary Conditions to Observation using Bayesian Nested Sampling* [In Preparation] [PDF Available on Request]

Contributing Author Publications

- Thomas, T.B., et al. (incl. **Gialluca, M.T.**), *Statistical geochemical constraints on present-day water outgassing as a source of secondary atmospheres on the TRAPPIST-1 exoplanets*. *PSJ* 6, 126. (2025)
- Barnes, R., et al. (incl. **Gialluca, M.T.**), *History and Habitability of the LP 890-9 Planetary System*. *PSJ*, 6, 25. (2025)
- Jenniskens, P., et al. (incl. **Gialluca, M.T.**), *Properties of outer solar system pebbles during planetesimal formation from meteor observations*. *Icarus*, 423, 116229. (2024)
- Jenniskens, P., et al. (incl. **Gialluca, M.T.**), *Lifetime of cm-sized zodiacal dust from the physical and dynamical evolution of meteoroid streams*. *Icarus*, 415, 116034. (2024)
- Buie, M.W., et al. (incl. **Gialluca, M.T.**), *Size and Shape of (11351) Leucus from Five Occultations*. *PSJ*, 2, 202. (2021)

Programming Experience

- **Python** – 9 years experience. *Familiar with packages including Matplotlib, Scipy, Astropy, Numpy, Keras & Tensorflow, Pandas, Multiprocessing, MPI via mpi4py, and more.*
- **Linux OS & Terminal Environment** – 9 years experience. *Terminal commands, shell scripting, and systems administration.*
- **LaTeX** – 8 years experience. *Used for all publications.*
- **Fortran** – 3 years experience. *Updating and modifying legacy code for atmospheric science (both F77 and F90); integrating Fortran-based models into Python data pipelines.*
- **LLM-Assisted Coding** – 1 year experience. *Familiar with the use of Claude, ChatGPT, and Gemini integration into programming workflow with Python*
- **C** – 2 years experience. *Modifying large collaborative [VPLanet codebase](#).*
- **MATLAB** – 1 year experience. *Translated MATLAB code to Python.*

Awards & Fellowships

- WA Space Grant Dissertation Completion Award for Outstanding Research & Outreach, \$6k (**Nov 2025**)
- Service to the UW Astronomy Dept Graduate Student Award, \$1k (**Fall 2025**)
- Private Donation from Autodesk for Astrobiology Program Outreach; \$20k Total in Donations (**Spring 2022 & Spring 2024**)
- NSF Graduate Research Fellowship; \$111k Total Stipend, \$44k Total Educational Allowance (**2021 – Present**)
- UW Provost Scholar Award for Academic Excellence, \$15k (**2021**)
- NAU Standard Bearer for College of Engineering, Forestry, and Natural Sciences (**2021**)
- Goldwater Scholarship, \$15k (**2019 – 2021**)
- NAU/NASA Space Grant for Research, \$2.5k (**2019 – 2020**)
- NAU Hooper Undergraduate Research Award, \$3.5k (**2018 – 2019**)
- NAU Presidential Tuition Scholarship, \$28k (**2017 – 2021**)
- National Young Astronomer's Award (**2016**)

Selected Service & Outreach

- **Lead Organizer, Astronomy on Tap** **Sept 2022 – Sept 2025**
Planning, delegating, and identifying speakers for the public outreach program Astronomy on Tap (AoT) Seattle. Collaborated with UW College of Arts and Sciences Marketing to create an [informational YouTube video on AoT](#).
- **Lead Organizer, UWAB Program 25th Anniversary Events** **Feb 2023 – April 2025**
Responsible for planning, marketing, and execution of public outreach events to celebrate the 25th Anniversary of the UW Astrobiology Program. Includes 2 single events and a Spring 2025 lecture series, which is [available on YouTube here](#).
- **Co-Founder & Leading Organizer, UW Raising eSTEAM** **Sept 2021 – Sept 2024**
One of the founding and leading members of the Raising eSTEAM team, a program dedicated to bringing education outreach and tutoring to incarcerated middle & high school students in Snoqualmie, WA. ([Raising eSTEAM website](#)) Single-handedly secured two \$10k private donations (\$20k total) to fund the program.
- **Member, Simulation Team for NASA Mission Ideation Factory** **Nov 2024**
Assisted with creating data and running simulated life-detection mission to Mars at NASA Ames.
- **Executive Secretary for NASA Habitable Worlds Proposal Evaluation Panel** **June 2024**
- **Executive Secretary for NASA ATP ROSES Panel** **Oct 2023**
- **Assisted with Securing NASA Virtual Planetary Laboratory ICAR ROSES Grant** **2022 – 2023**
PI: Prof Victoria Meadows. Grant was selected and funded \$7.5M (Grant No. 80NSSC23K1398)

Selected Academic Presentations

- Contributed Talk, Atmospheric Escape and Replenishment in Planetary Systems Workshop STSci (November 2025)
- Contributed Talk, Habitable Worlds Observatory Science Conference (July 2025)
- Invited Colloquium, University of Auckland (March 2025)
- Invited Colloquium, Victoria University of Wellington (March 2025)
- Invited Colloquium, University of Canterbury (March 2025)
- Contributed Talk, Astrobiology Science Conference [ABSciCon] (May 2024)
- Invited Presentation, Earth-Life Science Institute [ELSI] at the Institute of Science Tokyo (April 2024)
- Invited Presentation, National Astronomical Observatory of Japan [NAOJ] (April 2024)
- Poster Presentation, Extreme Solar Systems Conference (March 2024)
- Poster Presentation, Habitable Worlds Observatory Science Conference (July 2023)
- Poster Presentation, Statistics in Modern Astronomy Conference (June 2023)
- Contributed Talk, Oxygen in Planetary Biospheres Workshop (May 2023)
- Contributed Talk, AAS Conference (Jan 2023)
- Contributed Talk, Astrobiology Science Conference [ABSciCon] (May 2022)
- Contributed Talk, AAS Conference (2021) (Online due to COVID-19)
- Invited Talk, Harvard CFA REU Summer-end Symposium (2020) (Online due to COVID)
- Invited Talk, NASA Space Grant Symposium (2020) (Online due to COVID)
- Poster Presentation, NAU Student Research and Innovation Fair (2019)
- Poster Presentation, NAU Hooper Undergraduate Research Award (HURA) Reception (2019)
- Invited Talk, Astronomical League Convention (2016)