The Role of Atmospheric Exchange in False-Positive Biosignature Detection

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Key Points:

\begin{itemize}
\item The transfer of volatiles through atmospheric loss processes as seen in the Titan-Enceladus system may occur amongst close-in exoplanets
\item We simulate the atmosphere and spectra of TRAPPIST-1 e if it was receiving an external flux of water and oxygen
\item Our results are important for upcoming and future observatories which must prepare for false-positive biosignatures while searching for life
\end{itemize}

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Abstract
Saturn’s moon Titan receives volatiles into the top of its atmosphere - including atomic oxygen - sourced from cryovolcanoes on Enceladus. Similar types of atmosphere exchange from one body to another, such as O\textsubscript{2} and O\textsubscript{3} sourced from TRAPPIST-1 d, could be introduced into the upper atmosphere of TRAPPIST-1 e, and might be interpreted as biosignatures. We simulate this potential false positive for life on TRAPPIST-1 e, by applying an external influx of water and oxygen into the top of the atmosphere using a coupled 1-D photochemical-climate model (Atmos), to predict atmospheric composition. In addition, synthetic spectral observations are produced with the Planetary Spectrum Generator for the James Webb Space Telescope, Origins Space Telescope, Habitable Exoplanet Observatory and Large UV/Optical/IR Surveyor to test the detectability of abiotic-generated O\textsubscript{2} and O\textsubscript{3} in the presence of abiotic and biotic surface fluxes of CH\textsubscript{4}. We determine that the incoming flux of material needed to trigger detection of abiotic O\textsubscript{2}/O\textsubscript{3} by any of these observatories is more than two orders of magnitude \((1 \times 10^{12} \text{ molecules/cm}^2/\text{s})\) above what is physically plausible.

Plain Language Summary
In the Saturnian system, Enceladus’ icy volcanoes spew liquid and gasy material -including water- into outer space, and some of that material ends up in Titan’s atmosphere. This is a prominent phenomenon within our solar system that has been observed in great detail and shows proof of foreign matter exchange being possible between worlds. The simultaneous presence of detectable amounts of methane and oxygen or ozone in an atmosphere is considered strong evidence for the presence of life because in a methane rich atmosphere, oxygen or ozone will be destroyed to the point of being undetectable unless life is present to replenish it and vice-versa. We explore here whether a similar type of matter exchange, with methane present and occurring in the TRAPPIST-1 system, could increase oxygen and water abundances to the point of creating atmospheric signatures that may be mistaken for signs of life on another planet. To probe this question we use computer models of atmospheres and current and next-generation space telescopes. We conclude that when looking for the simultaneous presence of methane and oxygen/ozone, this matter exchange will not be mistaken for signs of life.

1 Introduction
As we move closer to being able to characterize the atmospheres of terrestrial exoplanets, the ability to identify signs of life and filter out false-positive biosignatures will be of the upmost importance. A biosignature is a detectable property of a planet (or environment) that results from the presence of life on a planet, and whose detection requires the presence of life (Lederberg, 1965; Lovelock, 1965; Marais & Walter, 1999; Des Marais et al., 2008; Schwieterman et al., 2018; Meadows et al., 2018). A false-positive biosignature is a means of producing such a detectable property via non-biological processes (Harman & Domagal-Goldman, 2018). Upcoming observatories have the potential to detect and characterize terrestrial planet atmospheres, and farther-off mission concepts plan to look for biosignatures (National Academies of Sciences & Medicine, 2021). Fauchez et al. (2020) have shown that for the TRAPPIST-1 planets in the habitable zone it will be challenging to detect water or any biosignature gas with the James Webb Space Telescope (JWST). However, carbon dioxide could be detectable and serve as a proxy to infer the presence of an atmosphere. NASA had four mission concepts evaluated for the Astro2020 Decadal Survey and three of them (Habitable Exoplanet Observatory, Origins Space Telescope and Large Ultra-violet Optical Infrared Surveyor - LUVOIR ) will be able to search for biosignatures on potentially habitable exoplanets (Gaudi et al., 2020; Cooray et al., 2019; LUVOIR, 2019). The relevant recommendations of the decadal survey were for a \(~6\text{m inscribed diameter Infrared/Optical/Ultraviolet space telescope with a}\)
target launch in the first half of the 2040s and a new Probe-class mission type to focus on a far-IR spectroscopy and imaging strategic mission (i.e. Origins) (National Academies of Sciences & Medicine, 2021). These recommendations, combined with the successful launch of JWST, motivate the continued study of biosignature and false-positive biosignature simulations in preparation for observational exoplanet atmosphere data in the near-term future. Prior work has argued that the presence of oxygen (and/or ozone, which is a photochemical byproduct of O$_2$) in combination with methane in an atmosphere is the most promising biosignature to look for (Hitchcock & Lovelock, 1967; Lovelock, 1975; Domagal-Goldman et al., 2014; Meadows, 2017). This classical “strong” biosignature pair of CH$_4$ and O$_2$/O$_3$ is considered robust due to their chemical interaction. In an atmosphere where O$_2$ is abundant and H$_2$O is present, the hydroxyl radical, OH, is produced which promotes the destruction of CH$_4$ by O$_2$ (Levy, 1971) while a CH$_4$-rich atmosphere would contain reducing sinks for O$_2$ that rapidly remove it from the atmosphere. This mutual destruction makes it difficult to maintain detectable levels of O$_3$ in the context of a CH$_4$-rich atmosphere without biological O$_2$ fluxes. Therefore the simultaneous presence of CH$_4$ and O$_3$ is an indicator of biological production of both CH$_4$ and O$_2$.

Biotic and abiotic sources of atmospheric CH$_4$ and O$_2$ on Earth have been extensively studied and can help constrain plausible flux ranges for this study. For example CH$_4$ can be produced as a metabolic byproduct of microbial life, and this process is evolutionarily ancient; putative evidence for this metabolism extends all the way back to 3.5 billion years ago (Ueno et al., 2006). And while Earth’s modern biosphere produces a biological CH$_4$ flux of $\sim$1×10$^{11}$ molecules/cm$^2$/s (Pavlov et al., 2001), estimates for the Archean range from $\sim$0.3-2.5 times this present-day value (Kharecha et al., 2005). CH$_4$ is also produced through geological processes, such as serpentinization, but at lower rates (Berndt et al., 1996). This means there is a range of potential CH$_4$ surface fluxes depending on whether they are produced abiotically or biotically (Arney et al., 2018) yet both of these forms potentially lead to accumulation of detectable CH$_4$ (Krissansen-Totton et al., 2016). This would complicate biosignature characterization efforts and require further context about the planet and host star to constrain the magnitude of the flux and understand its source (Krissansen-Totton et al., 2016; Arney et al., 2018).

As reviewed in Meadows (2017), O$_2$ has characteristics of a potential biosignature, but also has known, albeit specific and detectable, abiotic production mechanisms. These abiotic processes include slower O$_2$ and O$_3$ destruction on water (H$_2$O)-poor planets (Gao et al., 2015), fast O-production via photolysis on CO$_2$-rich planets around certain star types (Domagal-Goldman et al., 2014), and oxidation of the bulk atmosphere, driven by massive hydrogen escape on planets around pre-main sequence M-dwarfs (Luger & Barnes, 2015). Here we consider an additional potential source of O$_2$/O$_3$: an influx of O from space flowing into the top of the atmosphere (TOA) to form O$_2$ and O$_3$ abiotically.

Titan provides an example of such an inflow, and its impact on atmospheric chemistry. Titan exhibits rich photochemistry, which produces hydrocarbons, nitriles, and a haze of organic material (Brown et al., 2009; Niemann et al., 2010). Titan’s atmosphere is known to contain some oxygen, primarily CO. The origin of oxygen-bearing species in Titan’s atmosphere remained unresolved until the Cassini-Huygens mission. The Cassini Plasma Spectrometer detected a flux of O$^+$ ions into Titan’s atmosphere (Hartle et al., 2006), suggesting an external source for Titan’s oxygen-bearing species. The active, H$_2$O-rich plumes near Enceladus’ south pole (Porco et al., 2006) and its H$_2$O torus (Hartogh et al., 2011) provide a likely source. Dissociated and ionized H$_2$O molecules from the plumes are transported through the Saturn system supplying oxygen-bearing ions to Titan’s upper atmosphere. The precipitating O$^+$ ions participate in Titan’s photochemistry, and are likely responsible for the presence of CO, CO$_2$ (Hörst et al., 2008; Krasnopolsky, 2009), and perhaps even H$_2$O in Titan’s atmosphere (Hörst et al., 2008; Moreno et al., 2012).

Atmosphere loss and exchange processes between worlds could be amplified in planetary systems around very active M stars. In such systems, there is the potential for the
host star to strip away one planet’s atmosphere, leaving it inhospitable. The tight pack-
ing of systems like TRAPPIST-1 (Gillon et al., 2016, 2017) makes it possible for a larger portion of that lost atmosphere to be picked up by another close-by planet. Titan and Enceladus are approximately $10^6$ km apart, the same order of magnitude as the distance between TRAPPIST-1 d and e. In this work we study a scenario where an abiotic exoplanet receives an influx of water or atomic oxygen at the TOA from an outside source. Combined with an abiotic surface flux of CH$_4$, this creates the potential for both CH$_4$ and either O$_2$ or O$_3$ to be detected. If both are simultaneously detectable for reasonable incoming flux rates, this would represent a false-positive for an biosignature that has previously been considered to be “solid.” To investigate the potential for incoming exter-
nal fluxes into a terrestrial planet’s atmosphere to trigger a CH$_4$-O$_2$/O$_3$ biosignature false-
positive, we model the atmosphere of an abiotic planet exposed to varying exogenous fluxes of O or H$_2$O using the coupled photochemical-climate model, Atmos (Arney et al., 2016). We then use the Planetary Spectrum Generator (PSG,(Villanueva et al., 2018)) to sim-
ulate transit spectra for those atmospheres, and evaluate the detectability of O$_2$, O$_3$, and CH$_4$.

The paper is broken down into the following four sections. Section 2 explains the methods and tools used for the project, Section 3 is a presentation of our main data and most pertinent results, Section 4 is where we discuss our results and explain what they mean in the context of false-positive biosignatures and finally in Section 5 we tie every-
thing together into our conclusions.

2 Methods

2.1 Coupled Photochemical-Climate Modeling - Atmos

We use the coupled 1D photochemical-climate model, Atmos, to simulate the pho-
tochemistry and climate of TRAPPIST-1 e. The photochemical model was most recently
discussed in Arney et al. (2017) and Badhan et al. (2019). Here we use a version with
the updated wavelength grid from Lincowski et al. (2018). The model solves the contin-
uity and flux differential equations for the atmospheric species inputted and the solu-
tions correspond to a steady state atmosphere. Boundary conditions of the atmosphere
and parameters for the planet and host star are all adjustable by the user. For a given
atmospheric species, the lower boundary condition can be set to either a fixed deposi-
tion velocity, a constant surface flux, a constant flux distributed throughout the tropo-
sphere or a constant surface mixing ratio. For the upper boundary, a species can be as-
signed a constant TOA flux. In this project, we use the planetary parameters for TRAPPIST-
1 e from Agol et al. (2021) and assume an atmosphere with Earth pressure and abiotic
surface boundary conditions driven by redox balance (Harman et al., 2018; Domagal-Goldman
et al., 2014). The star and planetary parameters are listed in Table 1 and a list of the
species with non-zero boundary conditions can be found in Table 2. A complete list of
all species and boundary conditions is available in the supplemental material found in
the Zenodo data repository link in the acknowledgements section at the end of the pa-
per. These boundary conditions are paired with a photochemical reaction network, origi-
nally designed for Archean Earth (Arney et al., 2016) that has been expanded to include
more reactions and revised with updated reaction rate data. The applied stellar flux is
based on the semi-empirical PHOENIX model spectra of TRAPPIST-1 generated by Peacock
et al. (2019). We did not generate any appreciable haze since our largest CH$_4$/CO$_2$ ra-
tio was $4 \times 10^{-3}$, which is two orders of magnitude smaller than the 0.1 ratio at which
haze is expected to form for Archean Earth conditions (Trainer et al., 2006; Arney et
al., 2017). Although TRAPPIST-1 e is likely to be tidally locked (Kasting et al., 1993;
Barnes, 2017), we use a 1-D model which does not account for temperature and com-
position differences between the day and night side. To assess how inhomogeneous build-
up of O$_2$ due to tidal locking could affect the accuracy of our predictions, we perform

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Table 1: Host Star & TRAPPIST-1 e Planet Parameters

| Parameter          | Value     |
|--------------------|-----------|
| Host star          | TRAPPIST-1|
| Stellar type       | M8V       |
| Planet radius [R⊕] | 0.92      |
| Surface gravity [m/s²] | 8.01   |
| Surface pressure [bar] | 1.013   |
| Surface temperature [K] | 267     |
| Instellation [F⊕]  | 0.646     |

**Note.** Planetary parameters were taken from TRAPPIST-1 e (Agol et al., 2021). We assumed Earth-like surface pressure and the surface temperature is an average obtained from coupled photochemistry-climate simulations.

O₂ sensitivity scaling tests with our spectral simulator as described in Section 2.2 and Section 4.2.

To simulate an abiotic atmosphere we use abiotic boundary conditions from Harman et al. (2018). This approach assumes that in the absence of a biosphere, volcanic outgassing and reactions at the seafloor drive most of the chemical fluxes to/from the bottom of the atmosphere. To this set of boundary conditions, we add a surface CH₄ flux as well as TOA fluxes of either O or H₂O. We vary the CH₄, O, and H₂O flux values (Table 3), to see how the detectability of CH₄, O₂, and O₃ change in response to these fluxes. We follow Arney et al. (2018) and institute CH₄ fluxes (molecules/cm²/s) that are abiotic (1 × 10⁹), ambiguously abiotic or biotic (1 × 10¹⁰) and biotic (6 × 10¹⁰). These bins are consistent with probabilistic assessments of abiotic CH₄ fluxes from Krissansen-Totton et al. (2016).

The incoming O fluxes range from known examples in the Solar System on the low end to values that are on the threshold of what is likely to exist in nature on the high end. The lower limit of 1 × 10⁶ molecules/cm²/s is based on estimated oxygen flux into Titan’s atmosphere from Sittler et al. (2009) and the upper limit is taken from an exoplanet habitability study by Garcia-Sage et al. (2017). Garcia-Sage et al. (2017) simulated stellar induced ionospheric outflow of O⁺ from an Earth-twin of Proxima Centauri b, calculating the maximum O⁺ escape flux to be ∼10¹⁰ molecules/cm²/s. The high end of the range used in our study assumes maximum rates of atmospheric O loss from one terrestrial planet with perfect transfer of all material to a second planet. This type of “perfect transfer” is highly unlikely to occur in nature; so these high flux values represent an extreme end-member, to ensure that we bound all plausible incoming O flux values. For the scenario of an influx of water we follow the same pattern of establishing a lower and upper boundary.

Despite the implausibility of a water molecule surviving the trip from outer space and into an atmosphere wholly intact, we modelled the experiment this way for multiple reasons. First, there is the stoichiometric argument to be made that even if all of the water molecules were dissociated on their way to the top of a planet’s atmosphere, the hydrogen atoms should still be present. Second, using water molecules as a representation for oxygen molecule flux into an atmosphere is common practice by Titan photochemical modelers (Hébrard et al., 2012). Finally, by modelling a water flux we are able to account for other external oxygen sources to an atmosphere such as water ice (i.e. cryovolcanism on Enceladus). We set our incoming water flux lower bound at 5 × 10⁶ molecules/cm²/s based off of the work by Hébrard et al. (2012). The upper bound water flux is based on
estimated water loss on Earth, assuming perfectly efficient transfer of this water to a second planet. Similar to the upper end of our range of O fluxes, this is intentionally beyond the range of what we consider to be likely to occur in nature, as a means of ensuring that we have included all possible incoming H$_2$O flux rates. For both the O and H$_2$O flux there is the potential that neither of these scenarios will trigger a simulated O$_2$/O$_3$ signal. If this occurs we want to be able to quantify the fluxes needed to generate a false-positive. To prepare for this possibility we extend our simulations up to $1 \times 10^{12}$ molecules/cm$^2$/s.

The temperature-pressure profiles we use in this study are obtained by coupling the photochemistry model to the Atmos climate model. Derived from the 1D model created by Kasting and Ackerman (1986), the version of the climate code used here has undergone many updates (Kopparapu et al., 2013; Arney et al., 2016). The code uses the δ two-stream approximation (Toon et al., 1989) and absorption by the spectrally active gases - H$_2$O, O$_2$, O$_3$, CH$_4$ and C$_2$H$_6$ - is calculated based on the correlated-k method. The model’s H$_2$O and CO$_2$ k-coefficient have recently been recomputed using the HITRAN2016 database (Gordon et al., 2017). We use the Mega-MUSCLES TRAPPIST-1 spectral energy distribution from Wilson et al. (2021) for the climate model. In coupled mode, the photochemistry model passes the vertical mixing ratio profiles of the spectrally active gases and planetary parameters to the climate model. These are used by the climate model to compute the temperature-pressure profile and tropospheric water abundance which are in turn passed to the photochemistry model. The models iterate back and forth until both individual models are converged and a self-consistent atmospheric solution in radiative convective equilibrium is determined. For this study, we assume the tropospheric relative humidity parameterization by Manabe and Wetherald (1967). We run eight coupled photochemistry-climate simulations applying O$_2$, H$_2$O and CH$_4$ fluxes within the physically plausible range (Table 3). Subsequently, averaged temperature pressure profiles are computed and used as input for every photochemical simulation, see Fig. 1. Note that we are unable to arrive at a coupled solution for the boundary condition O flux $1 \times 10^{10}$ molecules/cm$^2$/s, CH$_4$ flux $1 \times 10^9$ molecules/cm$^2$/s and instead use the O flux $6 \times 10^9$ molecules/cm$^2$/s.
Table 2: Photochemical Model Boundary Conditions

| Species       | Boundary Type          | Value                      |
|---------------|------------------------|----------------------------|
| O             | \( \nu_{dep} \), downward flux | \( 1, 1 \times 10^6 - 1 \times 10^{10} \) |
| \( \text{O}_2 \) | \( \nu_{dep} \)         | \( 1 \times 10^{-4} \)    |
| \( \text{H}_2\text{O} \) | \( \nu_{dep} \), downward flux | \( 0, 5 \times 10^6 - 5 \times 10^{10} \) |
| H             | \( \nu_{dep} \)         | 1                          |
| \( \text{OH} \) | \( \nu_{dep} \)        | 1                          |
| \( \text{HO}_2 \) | \( \nu_{dep} \)      | 1                          |
| \( \text{H}_2\text{O}_2 \) | \( \nu_{dep} \)     | 0.5                        |
| \( \text{H}_2 \) | \( \nu_{dep} \), upward flux | \( 6.81 \times 10^{-6}, 1 \times 10^{10} \) |
| \( \text{CO} \) | \( \nu_{dep} \)         | \( 1 \times 10^{-8} \)    |
| \( \text{HCO} \) | \( \nu_{dep} \)        | 1                          |
| \( \text{H}_2\text{CO} \) | \( \nu_{dep} \)    | 0.1                        |
| \( \text{CH}_4 \) | upward flux            | \( 1 \times 10^9 - 6 \times 10^{10} \) |
| \( \text{CH}_3 \) | \( \nu_{dep} \)        | 1                          |
| \( \text{C}_2\text{H}_6 \) | \( \nu_{dep} \)      | \( 1 \times 10^{-5} \)    |
| \( \text{NO} \) | \( \nu_{dep} \)         | \( 3 \times 10^{-4} \)    |
| \( \text{NO}_2 \) | \( \nu_{dep} \)        | \( 3 \times 10^{-3} \)    |
| \( \text{HNO} \) | \( \nu_{dep} \)        | 1                          |
| N             | downward flux          | \( 1 \times 10^8 \)       |
| \( \text{H}_2\text{S} \) | \( \nu_{dep} \), upward flux | \( 0.015, 3 \times 10^8 \) |
| \( \text{HSO}_4 \) | \( \nu_{dep} \)       | 0.2                        |
| \( \text{SO}_2 \) | \( \nu_{dep} \)        | \( 3 \times 10^{-4} \)    |
| \( \text{CO}_2 \) | fixed mixing ratio     | 0.02                       |
| S             | \( \nu_{dep} \)        | 1                          |
| \( \text{HS} \) | \( \nu_{dep} \)        | \( 3 \times 10^{-3} \)    |
| \( \text{SO}_2 \) | \( \nu_{dep} \), upward flux | \( 1, 3 \times 10^9 \) |
| D             | \( \nu_{dep} \)        | \( 1 \times 10^{-2} \)    |
| \( \text{S}_8 \) Aerosol | \( \nu_{dep} \)     | \( 1 \times 10^{-2} \)    |
| \( \text{C}_4\text{H}_2 \) Aerosol | \( \nu_{dep} \)  | \( 1 \times 10^{-2} \)    |
| \( \text{C}_5\text{H}_4 \) Aerosol | \( \nu_{dep} \)  | \( 1 \times 10^{-2} \)    |
| \( \text{HNO}_2 \) | short-lived           |                            |
| \( \text{O}(^1\text{D}) \) | short-lived         |                            |
| \( \text{CH}_1^1 \) | short-lived          |                            |
| C             | short-lived            |                            |
| \( \text{SO}_2^1 \) | short-lived          |                            |
| \( \text{SO}_3^2 \) | short-lived          |                            |
| \( \text{HSO}_3 \) | short-lived          |                            |
| \( \text{OCS}_2 \) | short-lived          |                            |
| \( \text{CS}_2^* \) | short-lived          |                            |

**Note.** Species with non-zero boundary conditions used in the photochemical model. \( \nu_{dep} \) is the deposition velocity (cm/s) for a species. Downward flux (molecules/cm\(^2\)/s) is relative to the TOA, i.e. material entering the TOA from outer space, and upward flux is relative to the surface, i.e. material outgassing from the surface and moving up into the atmosphere. The multiple flux values for \( \text{O}, \text{H}_2\text{O}, \) and \( \text{CH}_4 \) correspond to the lower and upper physical limit values we impose. For a full list of boundary conditions, see the input files for our simulations at our Zenodo repository in the Acknowledgements section.
Table 3: Coupled Incoming Flux Combinations

| TOA flux     | CH₄ flux     |
|--------------|--------------|
| 1) Oxygen flux $1 \times 10^6$ | $1 \times 10^9$ |
| 2) Oxygen flux $1 \times 10^6$ | $6 \times 10^{10}$ |
| 3) Oxygen flux $1 \times 10^{10}$ | $6 \times 10^{10}$ |
| 4) Oxygen flux $6 \times 10^9$ | $1 \times 10^9$ |
| 5) Water flux $5 \times 10^6$ | $1 \times 10^9$ |
| 6) Water flux $5 \times 10^6$ | $6 \times 10^{10}$ |
| 7) Water flux $5 \times 10^{10}$ | $1 \times 10^9$ |
| 8) Water flux $5 \times 10^{10}$ | $6 \times 10^{10}$ |

**Note.** Flux input combinations used in the coupled photochemical-climate model runs.

Figure 1: Temperature profiles obtained with the coupled photochemistry-climate model (solid lines) and averaged (dash-dotted lines) temperature profiles for water (upper panel) and oxygen influx (lower panel). The two averaged temperature profiles are used for all of the photochemical and spectral simulations.
2.2 Synthetic Spectrum Generator - PSG

After all photochemical simulations are complete the vertical mixing ratio profiles of gases known to have an impact on terrestrial planet spectra - N$_2$, H$_2$O, CH$_4$, C$_2$H$_6$, CO$_2$, O$_2$, O$_3$, CO, and H$_2$CO - are sent as inputs to PSG, to produce synthetic transit spectra. PSG is an online radiative transfer tool (Villanueva et al., 2018) that uses a combination of radiative transfer models and spectroscopic databases to produce synthetic atmospheric spectra with either line-by-line calculations, the correlated-k method, or a combination of the two. For this project all spectroscopic data uses a combination of these two methods. Numerous types of planetary bodies (i.e. planets, exoplanets and comets) can be studied with PSG and we use it to simulate the transmission spectrum of our simulated planets as observed by four unique space-based observatories: JWST, Origins, HabEx and LUVOIR.

Clouds are prescribed in PSG based on TRAPPIST-1 e Archean Earth-like global climate model (GCM) simulations (Fauchez et al., 2019) using LMD-G GCM Wordsworth et al. (2011). Water and ice clouds are distributed between the surface and 19 km in the atmosphere profile. Water clouds, with a mass mixing ratio [kg/kg] of water droplets of 2 $\times$ 10$^{-6}$, range from the surface to 12 km and then ice clouds (mass mixing ratio [kg/kg] of ice droplets: 2 $\times$ 10$^{-7}$) are between 13 and 19 km. For every simulation with clouds, a clear sky case is also simulated.

From the photochemical-climate simulations we use the flux combinations #1, 3, 4, 5, 7 and 8 in Table 3. #1 and #5 are used to look for simulated detections of CH$_4$ at the lowest abundances, #3 and #8 probe for CH$_4$ and O$_2$/O$_3$ at the highest plausible ranges and #4 and #7 are used for O$_2$ sensitivity scaling tests. Since our simulations do not account for tidal locking and 3D GCM considerations (i.e. day-night side modeling), sensitivity tests on O$_2$ accumulation are performed with PSG. This consists of scaling the O$_2$ mixing ratio by a factor of 0.5, 2 and 10 and then analyzing the resulting spectra for O$_2$ features across every observatory. The scaling is performed uniformly throughout the atmosphere on O$_2$’s mixing ratio; N$_2$’s mixing ratio is set to maintain a total atmospheric pressure of 1 bar. To determine whether or not a signature is present and detectable by any of the four observatories a signal-to-noise ratio (S/N) has to be determined. This is dependent on tuning the resolving power of the instrument, for a specific signal (i.e. CH$_4$ at 7.72 $\mu$m), so that the resulting signal amplitude, continuum height, synthetic noise error bars and transmittance spectra provide the highest S/N.

Note that due to the successful launch of JWST, the amount of fuel present has been estimated to allow a 20 year lifetime. This is in contrast to the original 5.5 nominal lifetime pre-launch. We round this down to 5 years, and use the Contamination & Visibility Calculator tool (https://exoctk.stsci.edu/contam_visibility) to determine TRAPPIST-1 e will only be in the observing zone approximately a third of the time and so the system will be observable for 85 transits. We begin with 85 transits to compute the S/N for all telescope simulations and then an additional 1/$\sqrt{hv}$ scaling, where $hv$ is the number of photons, is applied to calculate 10 and 20 year lifetimes (170 and 340 transits respectively). An atmosphere profile and observatory are selected and given a resolving power (R) to start with, typically R=100. PSG is run and the resulting spectra are checked for CH$_4$, O$_2$ or O$_3$ signals. Non-overlapping features are identified and the best one is chosen based on the S/N. The S/N of the feature is calculated by subtracting the continuum from the features amplitude and then dividing that by the features synthetic noise. This provides an S/N value and then the resolving power is lowered from 100 in increments of 10 until the largest S/N is found. For all observatories, except JWST, we do not include their estimated noise floors and instead follow the procedure of Fauchez et al. (2019) and Pidhorodetska et al. (2020) by assuming a photon limited scenario where the noise is perfect and decreases with 1/$\sqrt{n}$, with $n$ being the number of transits. When JWST simulations are performed a noise floor of 10ppm is assumed. The observatory specific instruments and parameters are listed below. Note that although Origins, HabEx
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and LUVOIR have direct imaging capabilities we only simulate the instruments specific to observing exoplanets in transit.

1. Simulated JWST observations use two instruments: the Mid-Infrared instrument (MIRI) with the Low Resolution Spectroscopy (LRS) and the Near-Infrared Spectrograph (NIRSpec) with the Prism mode. MIRI-LRS observes in the 5-12 µm range and NIRSpec Prism is in 0.7-5 µm range. The MIRI-LRS configuration uses a resolving power of R=50 while NIRSpec Prism is set to 30 resolving power. MIRI-LRS has its S/N optimized by adjusting the resolving power, just as all of the other instruments do; R=50 gives the best results. We find this combination of instrument and transits to give the best resolution of our TRAPPIST-1 e hybrid while other scientists studying TRAPPIST-1 e with PSG (Fauchez et al., 2019; Pidhorodetska et al., 2020) have also used MIRI-LRS and NIRSpec Prism for simulating TRAPPIST-1 e transit observations.

2. For the Origins simulations we use the Transit Spectrometer of the Mid-Infrared Imager/Spectrograph/Coronagraph (MISC) Instrument in the 2.8-11 µm range with a resolving power of 30 (Cooray et al., 2019).

3. The HabEx simulations use the HabEx Work Horse Camera (HWC) with 30 resolving power in the 0.37-1.8 µm range (Gaudi et al., 2020).

4. The LUVOIR simulations are performed with the High Definition Imager (HDI) instrument, the block A mirror size (15 m) and a resolving power of 30 in the 0.2-2.5 µm range (LUVOIR, 2019). The Astro2020 Decadal Survey recommended a space observatory with a mirror that has a ~6m inscribed diameter, that would be a combination of the ideas and concepts laid out for LUVOIR and HabEx (National Academies of Sciences & Medicine, 2021). However, since our larger LUVOIR-A simulations do not produce a simultaneous CH₄ and O₂/O₃ detection it is unnecessary to also perform LUVOIR-B, or any architectures with smaller apertures, simulations.

3 Results

3.1 Atmos Results

Our coupled photochemical-climate model results appear in Fig. 2, 3, and 4. In Fig. 2 we display our mixing ratios for O₃, O₂, H₂O and CH₄. H₂O fluxes (top panel) have a more dramatic effect on the abundances of O₃, O₂, H₂O and CH₄, than the O fluxes (bottom panel). In the top panel a build up of H₂O in the upper layers of the atmosphere occurs, which is directly tied to the incoming TOA H₂O flux rising. Despite the large amount of incoming H₂O there was no super saturation in the top region of the atmosphere. When the CH₄ flux is low, increasing the water flux results in a higher percentage of O₃ and O₂ near the surface of the planet; when the CH₄ is high, varying the H₂O flux has little effect on the mixing ratios. This divergence between O₂ and O₃ surface mixing ratios, when water flux increases, is due to catalytic cycles between OH, HO₂ and H₂O₂ and increasing escape of H and H₂ from the atmosphere. The escaping H and H₂ diminish both the reducing power of the atmosphere and the strength of the catalytic cycle, thus removing O₂ sinks. As the water flux increases and the atmosphere is unable to maintain the catalytic cycle, O₂ builds up in the lower half of the atmosphere. This will only occur when the atmosphere crosses a redox threshold where it is becoming oxidized with time, which in the case of our simulations occurs when the water or oxygen TOA flux is greater than 1 × 10¹⁰ molecules/cm²/s, which is why the behavior is not seen in the bottom panel of Fig. 2. In the bottom panel the only noticeable changes occur when the CH₄ flux is varied, while the differences between low and high O flux are insignificant.
To show the effects of H\textsubscript{2}O and O fluxes on the whole atmosphere, we present CH\textsubscript{4} and O\textsubscript{3} column densities as a function of H\textsubscript{2}O flux (Fig. 3) and O flux (Fig. 4). As the incoming water and oxygen approaches the upper limit, the simulations show a gradual rise in O\textsubscript{3} densities while CH\textsubscript{4} densities remain completely static; the densities are not reacting strongly to the rising fluxes. The region on the far right of Fig. 3, and 4 shows the results when the physically plausible limits for water and oxygen fluxes are exceeded. It is important to note that these points past the limits are not included in the mixing ratio plots of Fig. 2. Only when this limit is breached do the simulated atmospheres begin to respond more sharply to the incoming oxygen and water. This is evident in the 1 to 3 order of magnitude changes in O\textsubscript{3} column densities for both water and oxygen fluxes. Conversely, the CH\textsubscript{4} is still responding slowly to the increasing fluxes (Fig. 3) or remaining unperturbed (Fig. 4).

Since our simulated atmospheres are receiving additional amounts of reducing and oxidizing material it is important to track the global ocean-atmosphere redox imbalance budgets to confirm redox is being conserved (Table 4 and Table 5). The redox imbalance represents the net reductant flux going into the atmosphere (+) or going into the ocean (-). We follow the methodology described in Harman et al. (2018) and our results show the global ocean-atmosphere redox for the boundaries of our parameter space and the flux combinations that are used in PSG. Our photochemical model is able to simulate modern day Earth conditions, an atmosphere with large biological methane and oxygen fluxes. We compare these modern day Earth ocean-atmosphere redox results to our influx simulations as a check for consistency.

Figure 2: Mixing ratios for O\textsubscript{3}, O\textsubscript{2}, H\textsubscript{2}O and CH\textsubscript{4} for the lowest and highest water fluxes and oxygen fluxes.
Figure 3: CH$_4$ and O$_3$ column density responses to increasing water flux values into the top of the atmosphere. The vertical dashed lines represent the lower and upper plausible limits of the water fluxes. The points to the right of the black vertical dashed line fall into the realm of physically implausible TOA fluxes. All data points use the average of the temperature profiles. Note the lack of data points for the red and purple dotted lines at water flux values $10^{10}$ and $5 \times 10^{10}$. These are regions where the photochemical model is not able to converge.

Figure 4: CH$_4$ and O$_3$ column density responses to increasing oxygen flux values into the top of the atmosphere. The vertical dashed lines represent the lower and upper limit of the oxygen fluxes.
Table 4: Coupled Model Global Ocean-Atmosphere Redox Imbalance Results - Water Flux

| H2O flux | CH4 flux | Ocean-Atmosphere Redox Imbalance |
|----------|----------|----------------------------------|
| $5 \times 10^6$ | $1 \times 10^3$ | $-9.48 \times 10^9$ |
| $5 \times 10^{10}$ | $1 \times 10^9$ | $7.66 \times 10^9$ |
| $5 \times 10^6$ | $6 \times 10^{10}$ | $4.61 \times 10^9$ |
| $5 \times 10^{10}$ | $6 \times 10^{10}$ | $2.24 \times 10^{10}$ |
| Modern Earth | $1 \times 10^{11}$ | $-2.95 \times 10^8$ |

**Note.** Global ocean-atmosphere redox values for the photochemical simulations that are coupled (Harman et al., 2018). The global ocean-atmosphere redox imbalance for the Modern Earth run with our photochemical model is also included as a reference for a world with large biological methane and oxygen fluxes.

Table 5: Coupled Model Global Ocean-Atmosphere Redox Imbalance Results - Oxygen Flux

| O flux | CH4 flux | Ocean-Atmosphere Redox Imbalance |
|--------|----------|----------------------------------|
| $1 \times 10^6$ | $1 \times 10^3$ | $-9.47 \times 10^9$ |
| $6 \times 10^3$ | $1 \times 10^9$ | $-3.56 \times 10^9$ |
| $1 \times 10^6$ | $6 \times 10^{10}$ | $4.63 \times 10^9$ |
| $1 \times 10^{10}$ | $6 \times 10^{10}$ | $1.463 \times 10^{10}$ |
| Modern Earth | $1 \times 10^{11}$ | $-2.95 \times 10^8$ |

**Note.** Coupled global ocean-atmosphere redox values when an oxygen flux into the TOA is present.

### 3.2 Synthetic Spectra Features - CH4, O3, O2

The first PSG-calculated molecule-detection signal/noise results appear in Table 6. This shows the S/N for all four observatories and their instruments under both, clear sky and cloudy conditions. We use the S/N as a metric to estimate the detectability of a given feature with a S/N of 5 being considered as reliable. And S/N is shown for 5, 10 and 20 year mission lifetimes. Due to the speculative nature of mission lifetimes beyond ∼5 years we only highlight the 5 year results here within the text as the baseline. The largest S/N for an atmosphere with clouds is produced for a LUVOIR-A HDI synthetic observation (19.05σ) and the relative transit depth (contrast) and transmittance spectra for this signal are shown in Fig. 5. This is a CH4 feature at 2.33 μm where the cloud opacity is weak in the transmittance and a TOA oxygen flux is present. Under clear sky conditions (Table 6), we predict that the following telescopes would detect a CH4 feature due to a S/N ≥ 5: Origins at 3.29 μm, JWST NIRSpec PRISM at 3.37 μm and LUVOIR at 2.33 μm. Under cloudy conditions only LUVOIR would detect a simulated CH4 feature (2.33 μm) due to a confidence level of at least 5σ. There were no instances of a simulated O3 or O2 feature detectable simultaneously with CH4 within the physical limit bounds we established. Our O2 sensitivity scaling test also returned null results for O2 or O3 S/N. The only observatory that showed a simulated feature was LUVOIR at 0.25 μm but the noise was extremely high (>500 ppm) resulting in a S/N less...
than 1. The extended mission lifetime scaling resulted in additional simulated CH\textsubscript{4} features with a S/N ≥ 5 but did not produce any reliable O\textsubscript{2} or O\textsubscript{3} features (Table 6).

### Table 6: CH\textsubscript{4}, O\textsubscript{2}, O\textsubscript{3} Detectability Results

| Observatory        | O flux | CH\textsubscript{4} flux | Cloudy CH\textsubscript{4} S/N | Clear Sky CH\textsubscript{4} S/N |
|--------------------|--------|---------------------------|---------------------------------|-----------------------------------|
| JWST MIRI-LRS      | 1 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 2.19, 3.09, 3.20                | 3.93, 5.55, 5.75                  |
| JWST NIRSpec PRISM | 1 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 2.34*                           | 5.02*                            |
| ORIGINS MISC-T     | 1 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 4.36, 6.17, 8.73                | 8.80, 12.45, 17.61                |
| HabEx HWC          | 1 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 1.47, 2.08, 2.95                | 4.93, 6.97, 9.86                  |
| LUVOIR-A HDI       | 1 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 19.05, 26.94, 38.11             | 34.79, 49.21, 69.59               |

| Observatory        | H\textsubscript{2}O flux | CH\textsubscript{4} flux | Cloudy CH\textsubscript{4} S/N | Clear Sky CH\textsubscript{4} S/N |
|--------------------|--------------------------|---------------------------|---------------------------------|-----------------------------------|
| JWST MIRI-LRS      | 5 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 2.18, 3.09, 3.20                | 3.87, 5.47, 5.67                  |
| JWST NIRSpec PRISM | 5 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 2.35*                           | 5.03*                            |
| ORIGINS MISC-T     | 5 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 4.38, 6.20, 8.77                | 8.83, 12.48, 17.66                |
| HabEx HWC          | 5 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 1.50, 2.13, 3.01                | 4.95, 7.00, 9.91                  |
| LUVOIR-A HDI       | 5 × 10\textsuperscript{10} | 6 × 10\textsuperscript{10} | 18.01, 25.47, 36.02             | 33.75, 47.73, 67.50               |

| Observatory     | O flux | CH\textsubscript{4} flux | O\textsubscript{2}, O\textsubscript{3} S/N | O\textsubscript{2}, O\textsubscript{3} S/N |
|-----------------|--------|---------------------------|--------------------------------------------|--------------------------------------------|
| All Observatories | 6 × 10\textsuperscript{9} | 1 × 10\textsuperscript{9} | -                                         | -                                         |

| Observatory     | H\textsubscript{2}O flux | CH\textsubscript{4} flux | O\textsubscript{2}, O\textsubscript{3} S/N | O\textsubscript{2}, O\textsubscript{3} S/N |
|-----------------|--------------------------|---------------------------|--------------------------------------------|--------------------------------------------|
| All Observatories | 5 × 10\textsuperscript{10} | 1 × 10\textsuperscript{9} | -                                         | -                                         |

**Note.** S/N results for all observatories studied. The S/N is computed for the *in transit* time only, without considering the out of transit observation and the values are for 85, 170 and 340 transits. The **bolded** values represent simulated detections with confidence levels of 5σ or higher. All O\textsubscript{3} and O\textsubscript{2} features are predicted to be non-existent, blended too heavily with other gases or completely enveloped by the synthetic noise. Flux is in units of molecules/cm\textsuperscript{2}/s. *Asterisk's denote JWST S/N values that triggered the estimated 10ppm noise floor in the first 5 years and thus are unable to improve their S/N with longer mission lifetimes (more transits).
Strongest Cloudy CH$_4$ Signal @ 2.33 µm – LUVOIR-A HDI

Transmittance Spectrum For Strongest Cloudy CH$_4$ Signal – LUVOIR-A HDI

Figure 5: Top Panel: Synthetic relative transit depth spectra of an atmosphere with an O TOA flux of $1 \times 10^{10}$ molecules/cm$^2$/s and a CH$_4$ surface flux of $6 \times 10^{10}$ molecules/cm$^2$/s. A potentially detectable CH$_4$ signal is simulated at 2.33 µm. Bottom Panel: The corresponding model transmission spectrum with the top four absorbers at 2.33 µm highlighted.

3.3 Synthetic Spectra - Incoming Oxygen & Water Past the Limits

Even though no O$_3$ or O$_2$ synthetic signal is produced within the bounds set in the column density plots from Fig. 3 and 4, we estimate how much O or H$_2$O flux is required to cause a potentially detectable O$_3$/O$_2$ signal. When the physical flux bounds were surpassed, simulated features appear within the wavelength range of JWST MIRI-LRS and LUVOIR-A but their transit depths and S/N are below the level of a reliable detection (Table 7). For JWST MIRI-LRS there is a simulated O$_3$ feature at $\sim$9.6 µm but the S/N is smaller than 5σ. Additionally, there is a 0.25 µm feature in LUVOIR-A’s wavelength
range; however, due to extreme noise in the UV the resulting S/N for this feature is less than 1σ. When the extended mission lifetimes are taken into account and the physically plausible flux ranges are breached, Origins MISC-T is able to simulate an O₃ feature at 9.73 µm with an S/N > 5 after 10 years (170 transits).

Table 7: Detections in Physically Implausible Flux Range

| Observatory       | O flux     | CH₄ flux | O₃ S/N | O₃ S/N |
|-------------------|------------|----------|--------|--------|
|                   | Cloudy     | Clear Sky|        |        |
| JWST MIRI-LRS     | 1 × 10¹²   | 1 × 10⁹  | 0.65, 0.92, 1.24 | 1.90, 2.69, 3.62 |
| JWST NIRSpec PRISM| 1 × 10¹²   | 1 × 10⁹  | -      | -      |
| ORIGINS MISC-T    | 1 × 10¹²   | 1 × 10⁹  | 1.00, 1.42, 2.01 | 3.03, 4.29, 6.07 |
| HabEx HWC         | 1 × 10¹²   | 1 × 10⁹  | -      | -      |
| LUVOIR-A HDI      | 1 × 10¹²   | 1 × 10⁹  | 0.09, 0.14, 0.19 | 0.14, 0.20, 0.29 |

Note. Synthetic simulations in the physically implausible parameter space from Fig 3 and 4. The CH₄ flux uses the abiotic value of 1 × 10⁹ molecules/cm²/s. Under these conditions, if the physically plausible flux ranges are breached and a mission lifetime extends past 10 years, then Origins MISC-T produces a synthetic O₃ observation, under clear sky conditions, with an S/N > 5.

3.4 Synthetic Spectra - Abiotic CH₄ Detections

At the abiotic CH₄ flux level (1 × 10⁹) we consider in our work, CH₄ features are present but all of them are at a S/N lower than 5σ and/or heavily blended with other gases such as H₂O and CO except when simulating ORIGINS MISC-T extended lifetime observations (Table 8). Under clear sky conditions we simulate ORIGINS detecting a 3.29 µm CH₄ with a S/N larger than 5σ. We also predict a simulated CH₄ feature in clear sky conditions for LUVOIR-A at 2.33 µm with a S/N over 21σ; however, the transmittance spectrum shows that this feature is predominately CO at 70%. No potentially reliable simulated feature was detected under cloudy conditions.
Table 8: CH$_4$ S/N For Lowest CH$_4$, H$_2$O & O Fluxes

| Potential Lifetimes [years] | O flux | CH$_4$ flux | CH$_4$ S/N | Clear Sky |
|-----------------------------|--------|-------------|------------|-----------|
| ORIGINS MISC-T              | 1 × 10^6 | 1 × 10^9  | -          | 4.16, 5.88, 8.32 |

Note. S/N CH$_4$ results when the CH$_4$ surface flux was 1 × 10^9 molecules/cm$^2$/s which is considered an abiotic flux. Using these fluxes, we predict that CH$_4$ is detectable under clear sky conditions in the extended lifetime scenario for ORIGINS MISC-T for both incoming flux types. **Bolded** values represent simulated detections with confidence levels of 5σ or higher.

4 Discussion

To avoid misidentifying biosignatures it is important to be aware of the many false-positives that can arise given the complexity of terrestrial exoplanets that we expect to encounter. We explored here whether the mechanism of volatiles flowing into a terrestrial planet’s atmosphere could produce a false positive by raising the levels of oxygen and ozone to abundances that would be misinterpreted as originating from biology. Our results indicate that this mechanism would not produce a detectable false-positive biosignature when observed by JWST or a next-generation observatory.

To simulate the incoming material flow of volatiles we needed to simulate a range of fluxes to the TOA. When doing so, we sought to set an aggressive value for the upper end of our flux range, to ensure our range of fluxes included all possible abiotic fluxes. We envisioned a scenario where a planet, such as TRAPPIST-1 d, orbiting an M dwarf was losing its atmosphere and that the next closest planet in the direction of the outflow was gaining it into their atmosphere, which in this case would be TRAPPIST-1 e. An M-dwarf system was chosen due to the ubiquitouness of M-dwarfs in the galaxy, the close-in region of the habitable zone around M-dwarfs and the tendency for increased stellar activity compared to G-stars which would lead to a higher chance of planets losing their atmospheres. Active M-dwarfs with their extreme ultraviolet output and flares are likely to increase atmospheric escape on any of their close-in planets causing the planets to lose their atmosphere. Even under such extreme assumptions, where every molecule outgassed from one planet ends up entering the second, we did not predict a detectable O$_2$/O$_3$ signal.

4.1 Oxygen & Water’s Role in Detectability

The results allow for a strong conclusion: fluxes of O into a planetary atmosphere will not lead to a detectable O$_3$ signal in an atmosphere that also has appreciable CH$_4$. The current understanding of O$_3$ detectability is that in atmospheres with detectable CH$_4$, O$_3$ will not be detectable for abiotic O$_2$ fluxes, which are significantly smaller than the O$_2$ flux from modern day biology ∼4 × 10^{13} molecules/cm$^2$/s (Walker, 1974). By considering that prior work and our results here, there is a consistent conclusion. Whether O is flowing into the atmosphere at the bottom or the top, the rates required to have O$_3$ accumulate to detectable levels in a CH$_4$-rich atmosphere are orders of magnitude higher than can be achieved through abiotic processes. Thus, gas fluxes - if they can be constrained - remain a very strong biosignature. Similarly, we predict water influxes will
not generate detectable O$_3$ concentrations. The incoming water flux does produce potentially detectable O$_3$ when extended mission lifetimes are considered but only at implausibly high fluxes. Thus, we can confidently say that an incoming water flux will not lead to a false-positive for the CH$_4$-O$_2$/O$_3$ biosignature pair.

4.2 Methane Detectability, Sensitivity Scaling of O$_2$ & Next Steps, JWST Scaling

Although this was not the main motivation for this study, we were also able to consider the impact of TOA H$_2$O and O fluxes on the detectability of CH$_4$. As Table 8 shows, we were able to predict the detection of a potentially reliable synthetic abiotic CH$_4$ feature when extended mission lifetimes were considered. Assuming an ORIGINS-like Probe-class mission is developed and launched, as the decadal survey recommends, then we can expect it to be able to detect abiotic amounts of CH$_4$ in a dry abiotic terrestrial atmosphere. Though LUVOIR-A saw a signal at 2.33 $\mu$m under clear sky conditions and the S/N was larger than 5$\sigma$, the issue becomes separating the signal into the CH$_4$ and CO components which already heavily favor the CO based on the transmittance results. If a desiccated (i.e. clear sky conditions) Earth-sized world was being observed and CO could be constrained then a next-generation observatory on the scale of LUVOIR-A may also be able to detect abiotic amounts of CH$_4$. This leads to the conclusion that neither JWST or any of the potential next-generation observatories could reliably detect abiotic CH$_4$ in a wet abiotic terrestrial atmosphere. Nevertheless, we urge caution in ascribing a biological source of CH$_4$ unless the CH$_4$ itself can be constrained to be at levels only consistent with a global biosphere.

Even though TRAPPIST-1 e is likely to be a synchronous rotator, by using a 1D model we negated the potential day and night side atmosphere discrepancies that could arise on such a body. However, our sensitivity scaling test on the accumulation of O$_2$ showed no effect on the detectability of this species. In addition, Chen et al. (2018, 2019) have shown that major atmospheric species of interest to our work (CH$_4$ and O$_3$) do not experience order of magnitude mixing ratio differences between the day and night side of tidally locked worlds orbiting active or quiescent M dwarfs.

While this study focused on the ability of TOA fluxes to create a “false positive” for life, additional studies may be performed to see how observations could detect and constrain the TOA fluxes. Such studies should make predictions of the observable impacts of this planetary process. This would allow future observatories to put these processes, observed on Titan, into a comparative planetology framework. The temperature profiles of our simulations could also be further improved with the coupling of a GCM. The inclusion of 1D climate coupling was a critical first step to simulating reasonable temperature profiles but the lack of cloud feedbacks on the temperature and atmosphere mean both the photochemical and spectral simulations can be further refined. Finally, we focused exclusively on space based observatories but next-generation ground based telescopes such as the European-Extremely Large Telescope (E-ELT) (Gilmozzi & Spyromilio, 2007), Giant Magellan Telescope (GMT) (Johns, 2006) and the Thirty Meter Telescope (TMT) (Skidmore et al., 2015) may also have a role to play in Earth-sized exoplanet characterization endeavors. This is highly dependent on the outcome of technological breakthroughs that are being tested at this time. For example, the E-ELT was recently upgraded as part of the New Earths in the Alpha Centauri Region (NEAR) campaign through the Breakthrough Initiatives. This upgrade consisted of experimental starlight suppression techniques while observing in the mid-infrared and the results currently stand at a potential minimum detection range of $\sim$3 Earth-radii (Carlomagno et al., 2020; Wagner et al., 2021). If this technology trend continues and the upcoming class of extremely large ground telescopes can reach smaller radii capabilities, then simulated false-positive biosignature detection comparisons between ground and space-based observatories would be an appropriate next step.
5 Conclusions

Our study shows that for transmission spectroscopy observations of terrestrial exoplanets orbiting M-dwarfs, the transfer of water or oxygen from one planet to another will not trigger a detectable false-positive for the biosignature consisting of the simultaneous presence of CH$_4$ and O$_2$/O$_3$ in a planetary atmosphere. The fluxes ($1 \times 10^{12}$ molecules/cm$^2$/s) required to do so would need to be more than two orders of magnitude larger than what abiotic processes would allow.

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DATA AVAILABILITY: All photochemical model runs, input files, and PSG configuration files are accessible at the public repository: Felton (2021).

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RCF performed all photochemical and PSG model runs, led analysis of the results and drafted the manuscript. SDDG helped conceptualize the project, and with STB provided guidance on the photochemical simulations and interpretations thereof, and provided feedback on the exoplanet and observatory implications of the work. STB also performed all coupled photochemistry-climate simulations. KEM and ALK provided insights into the transport of oxygen and water molecules in the Saturn system as well as guidance on determining reasonable upper limits for escape of heavy molecules from atmospheres. TJF provided inputs on the simulation of the transmission spectra and on the detectability of molecular signatures as well as on the observatories. Everyone contributed to the edits and comments of the entire manuscript.

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References
Agol, E., Dorn, C., Grimm, S. L., Turbet, M., Ducrot, E., Delrez, L., ... others (2021). Refining the transit-timing and photometric analysis of TRAPPIST-1: masses, radii, densities, dynamics, and ephemerides. *The planetary science journal*, 2(1), 1.
Arney, G., Domagal-Goldman, S. D., & Meadows, V. S. (2018). Organic haze as a biosignature in anoxic Earth-like atmospheres. *Astrobiology*, 18(3), 311–329.
Arney, G., Domagal-Goldman, S. D., Meadows, V. S., Wolf, E. T., Schwieterman, E., Charnay, B., ... Trainer, M. G. (2016). The pale orange dot: the spectrum and habitability of hazy archean earth. *Astrobiology*, 16(11), 873–899.
Arney, G., Meadows, V. S., Domagal-Goldman, S. D., Deming, D., Robinson, T. D., Tovar, G., ... Schwieterman, E. (2017). Pale orange dots: the impact of organic haze on the habitability and detectability of earthlike exoplanets. *ApJ*, 836(1), 49.
Badhan, M. A., Wolf, E. T., Kopparapu, R. K., Arney, G., Kempton, E. M.-R.,
Deming, D., & Domagal-Goldman, S. D.  (2019). Stellar activity effects on moist habitable terrestrial atmospheres around m dwarfs. *The Astrophysical Journal, 887*(1), 34.

Barnes, R.  (2017). Tidal locking of habitable exoplanets. *Celestial mechanics and dynamical astronomy, 129*(4), 509–536.

Berndt, M. E., Allen, D. E., & Seyfried Jr, W. E.  (1996). Reduction of co2 during serpentinitization of olivine at 300 c and 500 bar. *Geology, 24*(4), 351–354.

Brown, R., Lebreton, J. P., & Waite, H.  (2009). *Titan from cassini-huygens.* Springer Science & Business Media.

Carlolagno, B., Delacroix, C., Absil, O., Cantalloube, F., de Xivry, G. O., Pathak, P., . . . others (2020). Metis high-contrast imaging: design and expected performance. *Journal of Astronomical Telescopes, Instruments, and Systems, 6*(3), 035005.

Chen, H., Wolf, E. T., Kopparapu, R., Domagal-Goldman, S., & Horton, D. E.  (2018). Biosignature anisotropy modeled on temperate tidally locked m-dwarf planets. *The Astrophysical Journal Letters, 868*(1), L6.

Chen, H., Wolf, E. T., Zhan, Z., & Horton, D. E.  (2019). Habitability and spectroscopic observability of warm m-dwarf exoplanets evaluated with a 3d chemistry-climate model. *The Astrophysical Journal, 886*(1), 16.

Cooray, A., Meixner, M., Leisawitz, D., Staguhn, J., Armus, L., Battersby, C., . . . others (2019). Origins Space Telescope Mission Concept Study Report. *arXiv preprint arXiv:1912.06213.*

Des Marais, D. J., Nuth III, J. A., Allamandola, L. J., Boss, A. P., Farmer, J. D., Hoehler, T. M., . . . others (2008). The nasas astrobiology roadmap. *Astrobiology, 8*(4), 715–730.

Domagal-Goldman, S. D., Segura, A., Claire, M. W., Robinson, T. D., & Meadows, V. S.  (2014). Abiotic ozone and oxygen in atmospheres similar to prebiotic Earth. *The Astrophysical Journal, 792*(2), 90.

Fauchez, T. J., Turbet, M., Villanueva, G. L., Wolf, E. T., Arney, G., Kopparapu, R. K., . . . others (2019). Impact of clouds and hazes on the simulated JWST transmission spectra of habitable zone planets in the TRAPPIST-1 system. *The Astrophysical Journal, 887*(2), 194.

Fauchez, T. J., Villanueva, G. L., Schwieterman, E. W., Turbet, M., Arney, G., Pidhorydetska, D., . . . Domagal-Goldman, S. D.  (2020). Sensitive probing of exoplanetary oxygen via mid-infrared collisional absorption. *Nature Astronomy, 1–5.*

Felton, R.  (2021). Supplemental material: The role of atmospheric exchange in false-positive biosignature detection. zenodo. https://doi.org/10.5281/zenodo.5591912.

Gao, P., Hu, R., Robinson, T. D., Li, C., & Yung, Y. L.  (2015). Stabilization of CO2 atmospheres on exoplanets around M dwarf stars. *Astrophys J, 806*, 249–261.

Garcia-Sage, K., Glozer, A., Drake, J., Gronoff, G., & Cohen, O.  (2017). On the magnetic protection of the atmosphere of Proxima Centauri b. *The Astrophysical Journal Letters, 844*(1), L13.

Gaudi, B. S., Seager, S., Mennesson, B., Kiessling, A., Warfield, K., Cahoy, K., . . . others (2020). The Habitable Exoplanet Observatory (HabEx) Mission Concept Study Final Report. *arXiv preprint arXiv:2001.06683.*

Gillon, M., Jehin, E., Lederer, S. M., Delrez, L., de Wit, J., Burdanov, A., . . . others (2016). Temperate earth-sized planets transiting a nearby ultracool dwarf star. *Nature, 533*(7602), 221–224.

Gillon, M., Trifon, A. H., Demory, B.-O., Jehin, E., Agol, E., Deck, K. M., . . . others (2017). Seven temperate terrestrial planets around the nearby ultracool dwarf star trappist-1. *Nature, 542*(7642), 456–460.

Gilmozzi, R., & Spyromilio, J.  (2007). The european extremely large telescope (e-elt). *The Messenger, 127*(11), 3.
Gordon, I. E., Rothman, L. S., Hill, C., Kochanov, R. V., Tan, Y., Bernath, P. F., ... Zak, E. J. (2017, December). The HITRAN2016 molecular spectroscopic database. *JQSRT, 203*, 3-69. doi: 10.1016/j.jqsrt.2017.06.038

Harman, C. E., & Domagal-Goldman, S. (2018). Biosignature false positives. *Handbook of Exoplanets; Springer International Publishing AG, part of Springer Nature: New York, NY, USA, 71.

Harman, C. E., Felton, R., Hu, R., Domagal-Goldman, S. D., Segura, A., Tian, F., & Kasting, J. (2018). Abiotic O2 levels on planets around F, G, K, and M stars: effects of lightning-produced catalysts in eliminating oxygen false positives. *The Astrophysical Journal, 866*(1), 56.

Hartle, R., Sittler, E., Neubauer, F., Johnson, R., Smith, H., Crary, F., ... others (2006). Initial interpretation of Titan plasma interaction as observed by the Cassini plasma spectrometer: Comparisons with Voyager 1. *Planetary and Space Science, 54*(12), 1211–1224.

Hartogh, P., Lellouch, E., Moreno, R., Bockelée-Morvan, D., Biver, N., Cassidy, T., ... others (2011). Direct detection of the Enceladus water torus with Herschel. *Astronomy & Astrophysics, 532*, L2.

Hébrard, E., Dobrijevic, M., Loison, J.-C., Bergeat, A., & Hickson, K. (2012). Neutral production of hydrogen isocyanide (HNC) and hydrogen cyanide (HCN) in Titan’s upper atmosphere. *Astronomy & Astrophysics, 541*, A21.

Hitchcock, D. R., & Lovelock, J. E. (1967). Life detection by atmospheric analysis. *Icarus, 7*(1-3), 149–159.

Hörst, S. M., Vuitton, V., & Yelle, R. V. (2008). Origin of oxygen species in Titan’s atmosphere. *Journal of Geophysical Research: Planets, 113*(E10).

Johns, M. (2006). The giant magellan telescope (gmt). In *Ground-based and airborne telescopes* (Vol. 6267, p. 626729).

Kasting, J. F., & Ackerman, T. P. (1986). Climatic consequences of very high carbon dioxide levels in the Earth’s early atmosphere. *Science, 234*(4782), 1383–1385.

Kasting, J. F., Whitmire, D. P., & Reynolds, R. T. (1993). Habitable zones around main sequence stars. *Icarus, 101*(1), 108–128.

Kharecha, P., Kasting, J., & Siebert, J. (2005). A coupled atmosphere–ecosystem model of the early archean earth. *Geobiology, 3*(2), 53-76. Retrieved from https://onlinelibrary.wiley.com/doi/abs/10.1111/j.1472-4669.2005.00049.x doi: 10.1111/j.1472-4669.2005.00049.x

Kopparapu, R. K., Ramirez, R., Kasting, J. F., Eymet, V., Robinson, T. D., Mahadevan, S., ... Deshpande, R. (2013, March). Habitable zones around main-sequence stars: New estimates. *The Astrophysical Journal, 765*, 131. doi: 10.1088/0004-637X/765/2/131

Krasnopolsky, V. A. (2009). A photochemical model of Titan’s atmosphere and ionosphere. *Icarus, 201*(1), 226–256.

Krissansen-Totton, J., Bergsman, D. S., & Catling, D. C. (2016). On detecting biospheres from chemical thermodynamic disequilibrium in planetary atmospheres. *Astrobiology, 16*(1), 39–67.

Lederberg, J. (1965). Signs of life: criterion-system of exobiology. *Nature, 207*(4992), 9–13.

Levy, H. (1971). Normal atmosphere: Large radical and formaldehyde concentrations predicted. *Science, 173*(3992), 141–143.

Lincowski, A. P., Meadows, V. S., Crisp, D., Robinson, T. D., Luger, R., Lustig-Yaeger, J., & Arney, G. N. (2018). Evolved climates and observational discriminants for the Trappist-1 planetary system. *The Astrophysical Journal, 867*(1), 76.

Lovelock, J. E. (1965). A physical basis for life detection experiments. *Nature, 207*(4997), 568–570.

Lovelock, J. E. (1975). Thermodynamics and the recognition of alien biospheres.
An edited version of this paper was published by AGU. Copyright (2022) American Geophysical Union.
Skidmore, W., et al. (2015). Thirty meter telescope detailed science case: 2015. *Research in Astronomy and Astrophysics, 15*(12), 1945.

Toon, O. B., McKay, C. P., Ackerman, T. P., & Santhanam, K. (1989, November). Rapid calculation of radiative heating rates and photodissociation rates in inhomogeneous multiple scattering atmospheres. *Journal of Geophysical Research, 94*, 16287-16301. doi: 10.1029/JD094iD13p16287

Trainer, M. G., Pavlov, A. A., DeWitt, H. L., Jimenez, J. L., McKay, C. P., Toon, O. B., & Tolbert, M. A. (2006). Organic haze on Titan and the early Earth. *Proceedings of the National Academy of Sciences, 103*(48), 18035-18042.

Ueno, Y., Yamada, K., Yoshida, N., Maruyama, S., & Isozaki, Y. (2006). Evidence from fluid inclusions for microbial methanogenesis in the early archaean era. *Nature, 440*(7083), 516–519.

Villanueva, G. L., Smith, M. D., Protopapa, S., Faggi, S., & Mandell, A. M. (2018). Planetary spectrum generator: An accurate online radiative transfer suite for atmospheres, comets, small bodies and exoplanets. *Journal of Quantitative Spectroscopy and Radiative Transfer, 217*, 86–104.

Wagner, K., Boehle, A., Pathak, P., Kasper, M., Arsenault, R., Jakob, G., ... others (2021). Imaging low-mass planets within the habitable zone of α Centauri. *Nature communications, 12*(1), 1–7.

Walker, J. C. (1974). Stability of atmospheric oxygen. *American Journal of Science, 274*(3), 193–214.

Wilson, D. J., Froning, C. S., Duvvuri, G. M., France, K., Youngblood, A., Schneider, P. C., ... others (2021). The mega-muscles spectral energy distribution of Trappist-1. *The Astrophysical Journal, 911*(1), 18.

Wordsworth, R. D., Forget, F., Selsis, F., Millour, E., Charnay, B., & Madeleine, J.-B. (2011). Gliese 581d is the first discovered terrestrial-mass exoplanet in the habitable zone. *The Astrophysical Journal Letters, 733*(2), L48.