

Detectability of Atmospheric Climate and Biosignatures with the Large Interferometer for Exoplanets (LIFE) for Terrestrial-type Exoplanets

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ABSTRACT

We investigate the detectability of atmospheric biosignatures with the Large Interferometer for Exoplanets (LIFE) mission. Starting with the modern Earth we model the climate, photochemistry, and spectra of Earth-like planets over a range of insolation, gravity, humidity, albedo, atmospheric mass, and carbon dioxide abundances, and investigate detectability of key atmospheric species by LIFE for Earth-like planets assumed to lie at 10 pc for the LIFE (20-d viewing) baseline case. We find that atmospheric ozone (O_3) abundances are maintained over a range of conditions. The O_3 fundamental band is visible for most scenarios studied but is weakened for exoplanets with cooler central stars. Additional potential biosignatures such as methane (CH_4), nitrous oxide (N_2O), and chloromethane (CH_3Cl) have larger abundances for low UV conditions e.g. exoplanets orbiting cooler central stars or having strong atmospheric shielding. Regarding spectral signatures, CH_4 and water (H_2O) signals from 6–8 μm are evident in most scenarios, as is the carbon dioxide (CO_2) 15 μm band, which strengthens for low- O_2 scenarios associated with upper atmosphere cooling. Considering a 20-d viewing, H_2O is retrievable with a confidence level (CL) of 3.6σ for an Earth-like planet orbiting a cool star. N_2O is not observable with a CL sigma mostly less than one for the scenarios considered. CH_4 features a CL sigma detectability range of up to 1.5. O_3 is detectable in most cases with a CL of ~ 2.0 to 3.0 (including the low-ozone Proterozoic) except for the extremely low O_3 Archaean scenario and the low-pressure atmosphere scenario.

Key words: radiative transfer – telescopes – exoplanets – planets and satellites: atmospheres.

1. INTRODUCTION

The Large Interferometer for Exoplanets (LIFE) concept (S. Quanz et al., 2022) will herald in a new age regarding the search for life beyond the Solar system. The LIFE initiative proposes a space-based free-flying mid-infrared nulling interferometer concept with a 5- to 6-yr duration whose main aim is to characterize several dozen temperate rocky exoplanets in order to understand the diversity of habitable worlds and potential biosignatures. Correctly attributing signals as truly arising from biology requires theoretical studies that estimate the range and chemical origin(s) of the spectral signals to be measured (see e.g., J. Lederberg, 1965;

J. E. Lovelock, 1965; C. Sagan et al. 1993; S. Seager et al., 2013a). Numerical models are useful to simulate climate and biosignature responses to atmospheric environments (see e.g. F. Selsis et al., 2000; D. J. Des Marais 2002; V. S. Meadows et al., 2005; L. Kaltenegger et al., 2010) They are also useful when assessing the appropriate reporting framework for a potential biosignature detection (D. C. Catling et al., 2018; J. Green et al., 2021).

The field of remote atmospheric biosignatures on Earth-like planets has developed rapidly in the last few decades, as reviewed in J. L. Grenfell (2023). Numerous signals and/or processes have been proposed as potential biosignatures, including chemical redox disequilibrium, shifts in entropy production, shifts in chirality, and atmospheric spectral signatures (such as ozone) to name but a few (see e.g. the reviews in J. L. Grenfell, 2018 and E. W. Schwieterman and M. Leung, 2024). Here, we focus on the latter, namely atmospheric spectra for Earth-like biosignatures, and provide a short summary of related modelling studies.

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A seminal work modelling Earth-like atmospheres is J. F. Kast-
ing et al. (1993), who estimated the width of the habitable zone
(HZ) around main-sequence (F, G, K) stars. A. Segura et al. (2003)
subsequently modelled the photochemical responses for similar
planetary scenarios and noted that ozone (O_3) could mostly
maintain its abundance despite a reduction in its main source,
oxygen (O_2) by up to a factor of 1000, due to photochemical
responses conserving O_3 . In this sense, O_2 and O_3 are good biosig-
natures, although numerous works since then (e.g. R. Hu et al.,
2012; S. D. Domagal-Goldman et al., 2014; F. Tian et al., 2014; R.
Wordsworth and R. Pierrehumbert, 2014; R. Luger and R. Barnes,
2015) have investigated possible abiotic production scenarios for
these species (e.g. from CO_2 or/and H_2O photolysis followed by
H-escape) and have emphasized the importance of understand-
ing all atmospheric biosignatures in their particular environmen-
tal context (V. S. Meadows et al., 2018). L. Kaltenegger et al. (2007)
and S. Rugheimer and L. Kaltenegger (2018) discussed the evolu-
tion of atmospheric spectral signals from Earth-like planets over
geological eons. Results suggested that biosignature observability
is strongly suppressed by clouds and generally increases with
geological eon. S. D. Domagal-Goldman et al. (2011) performed
a model study that suggested that sulphur-containing biosigna-
tures such as dimethyl sulphide (DMS) (assuming an Earth-like
biomass) could build up to remotely detectable levels for young
rocky exoplanets orbiting cooler stars.

G. Arney et al. (2016) discussed the ability of atmospheric
organic aerosol to behave as a biosignature in Archaean-type
environments and suggested that such hazes could cool the sur-
face by up to 20 K. S. Seager et al. (2013b) investigated biosig-
nature responses in H_2 -dominated atmospheres of rocky exo-
planets, noting that ammonia (NH_3) and nitrous oxide (N_2O)
could be favoured biosignatures since they are not destroyed
by hydrogen sinks. D. Kitzmann et al. (2013) discussed the ef-
fects of clouds in rocky exoplanetary atmospheres; results sug-
gested that simple two-stream methods could significantly over-
estimate transmitted and reflected radiation compared with mul-
tiscattering techniques, especially for CO_2 ice clouds. J. L. Gren-
fell et al. (2013) simulated photochemical responses of biosig-
natures in the atmospheres of Super-Earths and noted a shift
from Chapman to smog ozone production on moving from Earth-
like planets orbiting successively cooler M-dwarf stars, due to
a weakening in the incoming UV flux. Numerous works mod-
elled Earth-like planets orbiting cooler stars including the ef-
fects of flaring and high energy particles (HEPs) (see e.g. A.
Segura et al., 2010; J. L. Grenfell et al., 2012; M. A. Tilley
et al., 2019; K. Herbst et al., 2019, 2024); the latter work, for
example, noted that nitric acid (HNO_3) could be a proxy for
Earth-like (N_2 - O_2 dominated) atmospheres in the presence of
HEPs since this species is produced photochemically in air
showers.

More recently there has been a move towards atmospheric
modelling of favoured low-mass host star exoplanet targets ob-
served by the James Webb Space Telescope (JWST) and fu-
ture concepts such as the Extremely Large Telescope (ELT)
and the Habitable Worlds Observatory (HWO). For example, M.
Scheucher et al. (2020) and N. Madhusudhan et al. (2020) per-
formed atmospheric modelling studies of the sub-Neptune K2-
18 b. Results suggested model predictions of habitability could
be sensitive to uncertainties in physical input parameters e.g.
in the deep convective region, as detailed in H. Innes and R. T.
Pierrehumbert (2022) and H. Innes et al. (2023). N. Madhusu-

han et al. (2023) recently suggested (weak) spectral evidence for
the potential biosignature, DMS, on K2-18 b, which has since
been contested (see e.g. O. Shorttle et al., 2024; S. M. Tsai et
al., 2024; J. F. Wogan et al., 2024; J. Taylor, 2025). Regarding
TRAPPIST-1e and f, F. Wunderlich et al. (2020) suggested that
dry and wet atmospheric scenarios could be distinguished with
 ~ 30 transits obtained by combining data from the JWST with
the ELT. R. Wordsworth and L. Kreidberg (2022) and T. Lichten-
berg and Y. Miguel (2025) reviewed favoured observing targets
for small rocky exoplanets, highlighting the potential diversity
of rocky exoplanet atmospheres. The former study (their table 1)
presented 11 favoured rocky targets with a Transit Spectroscopy
Metric of ~ 20 to 40. Recent model studies noted the importance
of consistent coupling between interior, surface, and atmosphere
for rocky exoplanets (L. Schaefer et al., 2016; R. D. Wordsworth
et al., 2018; T. Lichtenberg et al., 2021; P. Baumeister et al. 2023;
J. Krissansen-Totton et al. 2024), which is needed to better under-
stand atmospheric evolution. G. Ortenzi et al. (2020) presented
the first interior-atmosphere model study of its kind investigating
redox-dependent coupling and speciation.

Regarding 3D model studies, H. Chen et al. (2019) applied a
coupled climate-chemistry general circulation model (GCM) to
Earth-like planets around cooler stars, finding strong ozone loss
(hence changes in temperature and UV profiles) e.g. due to cat-
alytic destruction via hydrogen oxides, implying that constraints
on HOx and NOx reservoirs could be especially important under
such conditions, to correctly understand O_3 signals. H. Chen et
al. (2021) performed a 3D model study of the effect of flares on
tidally locked Earth-like planets; results suggested that H_2O and
 O_3 could be detectable with JWST for favoured rocky targets. G.
Cooke et al. (2023) used the whole atmosphere version of the
Community Atmosphere Model version 6 (WACCM6) to examine
how observer angle, albedo, chemistry, and clouds impact the
detectability of oxygen with HWO. The GCM study by M. J. Way
et al. (2018) noted that the choice of ocean transport module
and assumed planetary rotation rate are potentially important
factors for the habitability of Earth-like planets. M. Godolt et al.
(2016) suggested that 1D models can broadly reproduce habitable
conditions predicted by 3D models, assuming surface properties
and relative humidity are reasonably well known.

Regarding the LIFE mission, numerous works have discussed
the mission concept (S. Quanz et al., 2022), scientific require-
ments (B. S. Konrad et al., 2022; A. Glauser et al., 2024), design (J.
T. Hansen et al., 2022, 2023), and detectability of exoplanets (Ó.
Carrión-González et al., 2023; L. Cesario et al., 2024). E. Alei et al.
(2022) studied detectability of atmospheric biosignatures by LIFE
for different eons based on Earth's evolution. D. Angerhausen et
al. (2024) discussed biosignature detectability for model scenar-
ios based on modern Earth, varying biomass emissions and the
central star, suggesting detectability of a few sigma for e.g. nitrous
oxide (N_2O) at 5 pc. B. Taysum et al. (2024) discussed detectability
of key atmospheric species assuming warm Earth-like planets.

In this work we perform simulations of scenarios that start
with the modern Earth and then vary key parameters (atmo-
spheric composition and mass, host star, planetary orbit, surface
albedo, etc.). We apply our recently developed photochemistry-
climate model 1D-TERRA, which has been validated for modern
Venus, Earth, Mars, and Titan (M. Scheucher et al., 2020; F. Wun-
derlich et al., 2020) and applied to a wide range of atmospheric
conditions investigating rocky exoplanets. We present a chemical
analysis of the biosignature responses, calculate infrared emis-

sion spectra with the GARLIC model (F. Schreier et al., 2014), apply instrument noise using the LIFE signal simulator, LIFE_{SIM} (F. A. Dannert et al., 2022), and finally apply two retrieval models. First, a straightforward retrieval approach based on the Differential Optical Absorption Spectroscopy (DOAS) method (see Section 2.5) to obtain atmospheric trace gas column densities for nine key species, corresponding to the vertical column from the top-of-atmosphere down to the emitting layer when the planetary emission lies directly in the line of sight. Secondly, the SVEETIES (Singular Vector Expansion to Estimate Earth-like Exoplanet Temperatures from Infrared Emission Spectra) model to retrieve atmospheric temperature profiles (see Section 2.6).

2. DESCRIPTION OF METHODS AND MODELS

2.1 The LIFE mission concept

The LIFE baseline architecture currently considered consists of the so-called X-array configuration with four collector spacecrafts in a rectangular array that send light to a beam combiner spacecraft in the centre. The configuration is rotated around the line of sight, which results in the fringe pattern also rotating hence modulating the planet signal as it moves through the fringe pattern. Since the array is free-flying the baseline can be adjusted depending on the required spatial extent of the fringe pattern. Aperture diameters (D) varying from $D = 1$ m to $D = 3.5$ m are under investigation for a ‘standard’ wavelength range of 4–18.5 microns (emission) spectra. Assuming $D = 2$ m and a 5 per cent throughput is estimated to yield 391–586 exoplanets (having 0.5–6.0 Earth radii and orbiting F, G, K stars) depending on the observing strategy and with input based on exoplanet occurrence statistics from the Kepler mission (for more details see S. Quanz et al., 2022, their fig. 5). For a recent description of the mission baseline concept see A. Glauser et al. (2024).

2.2 Atmospheric column model: 1D-TERRA

1D-TERRA is a 1D stationary cloud-free global-mean climate-photochemical atmospheric model extending from the planetary surface up to the lower thermosphere. The climate and chemistry modules have 100 model layers each with ~ 1 km thickness. The model is valid over a broad range of atmospheric compositions and masses (M. Scheucher, 2021). The climate module operates over pressures ranging from 1.3×10^{-7} to 1000 bar and temperatures from 100 to 1000 K. Future climate module versions simulating the higher temperature end ($T > 800$ K) of this range (see M. Scheucher et al., 2020) are planned to be tested although this effect is not significant for the cooler scenarios considered here. The chemistry module operates over pressures ranging from 1.3×10^{-7} to 100 bar and temperatures below 800 K. 1D-TERRA validations are further discussed in M. Scheucher et al. (2020) for the climate module and in F. Wunderlich et al. (2020) for the chemistry network.

2.2.1 Climate module

The climate module uses the correlated-k approach to solve the radiative transfer equation by considering wavelengths from 0.1 to 1000 microns with up to 20 main absorbers based on the HITRAN 2016 linelist (I. Gordon et al., 2017) and 81 absorbers covering the far ultraviolet (FUV) ($121.5 < \lambda < 175$ nm) to the

visible wavelength range based on the MPI Mainz Spectral Atlas (H. Keller-Rudek et al., 2013), which can be adapted flexibly by the user. The climate module includes a range of collision-induced absorption (CIA) data and employs a Rayleigh extinction parametrization for eight molecules. The convergence criteria require a change of (1) less than 0.1 K in temperature and (2) less than 1 milliwatt in radiative flux over two consecutive iterations throughout the entire profile for a time-step larger than one Earth day. Starting with a purely radiative profile the climate module applies the Schwarzschild criterion from the surface upwards in order to determine the convective upper boundary (tropopause). In the convective region the model applies an adiabatic lapse rate and calculates the water vapour profile based on relative humidity values from S. Manabe and R. T. Wetherald (1967). Further details can be found in M. Scheucher et al. (2020).

2.2.2 Photochemistry module

The chemical network of the planetary atmosphere features 1127 chemical reactions for 128 species including all major carbon, hydrogen, oxygen, nitrogen, sulphur, and chlorine-containing species. Surface fluxes (molecules $\text{cm}^{-2} \text{s}^{-1}$) in the control run were fixed to $\text{CH}_4 = 1.4 \times 10^{11}$, $\text{N}_2\text{O} = 1.4 \times 10^9$, $\text{CH}_3\text{Cl} = 2.2 \times 10^8$, $\text{CO} = 2.2 \times 10^{11}$, and $\text{H}_2 = 9.3 \times 10^{10}$. Long-lived trace gases (vmr) in the control run were fixed to $\text{O}_2 = 0.21$, $\text{CH}_4 = 0.78$, and $\text{CO}_2 = 3.3 \times 10^{-4}$. Photolysis reactions are present for 81 species with radiative fluxes in 133 bands from 100 to 850 nm for a geometrical mean solar zenith angle to reproduce the global average. The photochemical rate coefficients are taken mainly from J. Burkholder et al. (2015) and the National Institute of Standards and Technology (NIST, W. G. Mallard et al. 1994). Chemical tendencies are obtained by treating the network as a series of differential equations that are integrated with a Euler backward stepping method whose iteration step is variable depending on the stiffness of the system. Eddy mixing is calculated as described in F. Wunderlich et al. (2020). Incoming HEP can be calculated with the Gaiser–Hillas method with further details in J. L. Grenfell et al. (2007). The convergence criteria require a change of less than 10^{-20} in species abundance over two consecutive iterations for all species over the entire model domain for an iteration step larger than one Earth year. More details on the photochemical network can be found in F. Wunderlich et al. (2020).

2.3. Line-by-line spectral models: GARLIC and Py4Cats

The Generic Atmospheric Radiation Line-by-line Infrared Code (GARLIC) is used to calculate synthetic emission and transmission spectra (see F. Schreier et al., 2014; 2018). Line parameters are based on HITRAN 2016 (I. Gordon et al., 2017). In addition to the lbl molecular absorption the parametrization includes the (Mlawer–Tobin–) Clough–Kneizys–Davies continuum model ((MT)CKD; S. Clough et al., 1989; E. Mlawer et al., 2023) for water vapour and Rayleigh extinction (W. F. Murphy 1977; S. Clough et al., 1989; M. Snee & W. Ubachs 2005; E. Marcq et al., 2011). Emission spectra are computed for a nadir geometry assuming a fixed viewing angle. The corresponding flux can be obtained by scaling with π . Absorption (effective height) spectra are calculated for 100 tangential beams (corresponding to the 100 layers in the 1D-TERRA chemistry) throughout the atmo-

sphere. Absorption spectra here used the CKD CIA and H₂O-continuum with O₂ N₂ CO₂ CIA. The Py4CATS (Python for Computational Atmospheric Spectroscopy) is a (Numeric) Python re-implementation of GARLIC (F. Schreier et al., 2019) available at <https://atmos.eoc.dlr.de/tools/Py4CATS/index.html> and serves as forward model for the temperature retrievals discussed in Sections 2.6 and 4.4.3.

2.4 LIFE noise simulator: LIFE_{SIM}

LIFE_{SIM} is a software tool for simulating exoplanetary observations with an MIR interferometer. LIFE_{SIM} calculations in this work are based on emission spectra input calculated by GARLIC (see Section 4.2). The package includes photon noise, stellar leakage, and thermal emission noise from local zodiacal and exozodiacal dust and is designed flexibly such that instrument noise can be added as additional design parameters become available. Photon noise is calculated from the Planck equation assuming the stellar disc to be a blackbody with uniform brightness (no limb darkening). Stellar leakage (which arises since the stellar flux is not completely suppressed by instrumental nulling) is calculated by applying transmission maps to the stellar surface area. Local zodiacal dust is parametrized using thermal data from the COsmic Background Explorer (COBE) Mission (T. Kelsall et al., 1998). Exozodiacal dust is based on the model described in G. M. Kennedy et al. (2015) and assumes a distribution similar to the Solar system except for a global scaling factor, z (the number of zodis) where $z = 3$; this value is consistent with the HOSTS (Hunt for Observable Signals of Terrestrial Systems) survey (S. Ertel et al., 2020). The model assumes face-on surface density of the dust approximated by a power law with emission calculated assuming a blackbody. We assumed a detector quantum efficiency, $\eta_{QE} = 0.7$ and instrument throughput, $\eta_t = 0.05$. Further details of LIFE_{SIM} can be found in F. A. Dannert et al. (2022).

2.5 Atmospheric column retrieval algorithm: composition

Column densities of key atmospheric trace species are retrieved with a technique analogous to the DOAS method (U. Platt and J. Stutz, 2008) widely used in remote sensing of the terrestrial atmosphere (e.g. M. Buchwitz et al., 2000). From the observed radiances, I_{obs} , as well as the Planck curve radiance, $I_{surface}$ (corresponding to an assumed surface temperature), we derive the atmospheric optical density, τ_{atm} , as a function of wavelength via

$$\tau_{atm} = -\ln\left(\frac{I_{obs}}{I_{surface}}\right) = \sum \sigma_i X_i \quad (1)$$

Here, we take a surface temperature of 300 K as a reasonable assumption for an Earth-like planet; for real observations, an estimate of the surface temperature could be derived from the broad-band shape of the observed Infrared radiances in regions without strong absorption features. The optical density is a linear function of the trace gases column densities X_i (i = species number, X = column density), which can then be fitted with a simple multilinear regression, where the regressors are the absorption cross-sections of the fitted trace gases (σ_i in equation 1). Here, we consider only absorption features of the strong IR emitters: CO₂, H₂O, CH₄, O₃, HNO₃, N₂O and SO₂. NO, NO₂, and CO were tested, but did not yield significant results for the scenarios used here. To account for unresolved absorption features with a long-wavelength dependence such as Mie scattering of aerosols or clouds, a polynomial of degree three is fitted as well. The

advantage of this rather simple method is that it is very robust. Also, it does not emulate any information which is not inherent in the observations, such as information on altitude profiles, and it does not need any regularization or a priori information; all the information gained depends on the observation alone.

Since the atmospheric amount of short-lived trace gases like O₃, HNO₃, or NO₂ could vary greatly between the illuminated and dark atmospheres, which are both within the field of view in varying amounts, lower denser parts of the atmospheres might be optically dense, and the assumption of a constant atmospheric temperature and pressure would imply errors in the retrieval. Hence the absolute column density values retrieved with this method are likely to be only rough estimates. However, the resulting average vertical column densities of the lower pressure upper atmosphere together with their retrieval error provide a robust estimate on the significance of the detected absorption features of the trace gases.

The absorption cross-sections are generally temperature- and wavelength-dependent, which has to be taken into consideration when determining the column densities e.g. by fitting the line shapes. Since however the spectrum we see is integrated over the whole atmospheric column, i.e. averaged over a range of pressures and densities, and employs a somewhat limited spectral resolution, such a fitting procedure is not possible with great accuracy, and we do not attempt to do this here, although it should be pointed out that this might yield interesting results with real-world data. We use absorption cross-sections for a pressure of 1000hPa and a temperature of 300 K, which we take as a reasonable assumption for a moderately thick (Earth-like) atmosphere. The square of the measurement noise forms the diagonal elements of the error covariance matrix, ensuring that the retrieval is sensitive to regions with a low signal-to-noise ratio. This also enables us to calculate the error covariances of the retrieval results, and the significance of the retrieval for the different trace species is provided as the ratio of the retrieved column density to its retrieval error.

2.6 Atmospheric profile retrieval algorithm: temperature

For the sounding of atmospheric temperature profiles, we use the non-linear least squares solver coupled to Py4CATS (F. Schreier et al., 2019). Temperature is represented as a superposition of Chebychev polynomials with unknown expansion coefficients similar to the SVEEEETIES study (F. Schreier et al., 2020). Synthetic thermal IR emission ‘observations’ are generated by convolution of monochromatic radiance spectra with a Gaussian response function of constant half width and injected with noise ($S/N = 10$). Molecular line-by-line data are taken from HITRAN 1986 (L. S. Rothman et al., 1987) and from Earth climatological data (G. P. Anderson et al. 1986).

3. SCENARIOS: MOTIVATION AND BACKGROUND

We performed in total 22 scenarios. Our main motivation here is to explore changes in key stellar, planetary, and atmosphere properties starting with the modern Earth. The range of variation is based on knowledge of the evolution of the rocky planets in the Solar system and on previous modelling studies of Earth-like planets. For each scenario we investigate the effect of only one change at a time.

Table 1 summarizes the 22 scenarios performed. Scenario 1 is

Table 1. Overview of 22 model scenarios performed.

Scenario number	Scenario name	Description
1	Earth Control	Modern Earth around the Sun
2	Dark Earth	Halved surface albedo
3	Bright Earth	Doubled surface albedo
4	+10 per cent insolation	Insolation increased by 10 per cent
5	−10 per cent insolation	Insolation decreased by 10 per cent
6	Dry Earth	Low surface humidity
7	2 g Earth	Doubled gravity
8	3 g Earth	Tripled gravity
9	100mb P_0	0.1 bar surface pressure
10	2 bar P_0	2 bar surface pressure
11	5 bar P_0	5 bar surface pressure
12	10 bar P_0	10 bar surface pressure
13	1 per cent CO_2	1 per cent (0.01 vmr) CO_2
14	10 per cent CO_2	10 per cent (0.1 vmr) CO_2
15	20 per cent CO_2	20 per cent (0.2 vmr) CO_2
16	50 per cent CO_2	50 per cent (0.5 vmr) CO_2
17	90 per cent CO_2	90 per cent (0.9 vmr) CO_2
18	Proterozoic	‘Earth’ with Proterozoic O_2
19	Archaean	‘Earth’ with Archaean O_2
20	GJ832	‘Earth’ orbiting GJ832
21	ADLeo	‘Earth’ orbiting AD Leonis
22	ProxCen	‘Earth’ orbiting Proxima Centauri

the modern Earth control with greenhouse gases and biomass emissions set to 1990 levels, surface albedo = 0.259 and mean incoming solar insolation (see F. Wunderlich et al., 2020 and references therein for further details). Scenario 2 features a halved surface albedo (=0.1295) compared with the control scenario, whereas in scenario 3 this value is doubled (=0.518). These are modest changes compared to the envisageable range from dark (e.g. basalt = 0.11) to light (e.g. fresh snow = 0.85) surfaces. These two values represent rather extreme end member cases and the surface albedos assumed in our 22 scenarios (Table 1) lie in this range.

Scenarios 4 (and 5) feature a 10 per cent increase (decrease) in the wavelength-integrated, top-of-atmosphere (TOA) insolation compared with the control scenario. These values are based on J. L. Grenfell et al. (2007) and correspond to the modelled limits of the complex life HZ ($T_{\text{surface}} = 0$ to 30°C in the global mean) for a planet with Earth’s properties. Scenario 6 features surface relative humidity (per cent RH) decreased from the global mean value of 80 per cent (S. Manabe and R. T. Wetherald, 1967) in the Earth control to 1 per cent (and the tropospheric humidity profile scaled accordingly). A value of 1 per cent RH occurs only rarely in Earth’s driest regions such as at the South Pole; such a value was also assumed for the ‘dry case’ in F. Wunderlich et al. (2020).

Scenario 7 (and scenario 8) simulate Super-Earths by introducing doubled (and tripled) gravity respectively. These scenarios simulate a planet with Earth’s mean density but twice (three times) the radius, leading to twice (three times) Earth’s gravity respectively, on considering the change in mass together with Newton’s universal gravity law. The upper radius limit for a rocky planet lies between 2 and 3 Earth radii, but likely nearer the lower end of this range (e.g. H. Parviainen et al., 2024). On varying gravity in atmospheric models, there are commonly two approaches: either (a) assume constant surface pressure, then the atmospheric column value (in molecules cm^{-2}) decreases linearly with gravity, or (b) assume a constant atmospheric column, then the surface pressure has to be increased to counter the enhanced gravity; scenarios 7 and 8 assumed the former.

For scenarios 9 to 12, the surface pressure is varied while approximately maintaining the same $\text{N}_2 : \text{O}_2$ ratio as in the Earth control scenario. To achieve this, first the desired, initial pressure (P_0) is set (e.g. $P_0 = 100\text{mb}$ in scenario 9). Initial $\text{O}_2 = 0.21$ volume mixing ratio (vmr) as in the modern Earth scenario. The minor species, including H_2O are also held at the same initial values as the Earth control. Finally, N_2 is set to be the ‘fill gas’ i.e. it is added appropriately such that the initial $P_0 = 100\text{mb}$. In the converged scenario, minor species can deviate from the initial values due to responses in the chemistry and climate due to the changed P_0 ; these changes, however, are minor compared with contribution of the total vmr to the fixed, surface N_2 and O_2 ; in this sense, scenarios 9 to 12 have modern Earth-like $\text{N}_2\text{--O}_2$ abundances.

Scenarios 13 to 17 vary the CO_2 abundance from 0.01 to 0.9 vmr while maintaining initial $P_0 = 1$ bar, N_2 as fill gas and $\text{O}_2 = 0.21$ vmr except for the 0.9 CO_2 vmr scenario where $\text{O}_2 = 10^{-5}$ vmr. Regarding rocky exoplanets across the HZ, CO_2 abundances are anticipated to be stabilized due to the carbonate-silicate cycle, which is challenging to simulate; the model study by O. R. Lehmer et al. (2020) suggests CO_2 abundances of up to ~ 10 bar on simulating ‘Earth’ moved to Mars’ orbit. Based on the empirical HZ in the Solar system, the inner (outer) limits marked by modern Venus and Mars suggest strongly CO_2 -dominated atmospheres with a few per cent N_2 , etc. In summary, the range of CO_2 vmr taken in our study appears reasonable based on the available data.

Scenario 18 features surface O_2 reduced by a factor 100, appropriate to Proterozoic conditions (D. C. Catling and M. W. Claire, 2005). Scenario 19 has surface O_2 reduced to 10^{-5} vmr appropriate to mid-Archaean conditions (D. C. Catling and M. W. Claire, 2005). Note that since we vary only one effect at a time, the two Early Earth scenarios (18 and 19) only feature the oxygen change, not a change in other factors such as the solar constant compared with the Earth Control scenario.

Scenario 20 simulates ‘Earth’ in orbit around GJ832 (M1.V) where it receives the same net instellation as the modern Earth scenario (see F. Wunderlich et al., 2020 for details on deriving

Table 2. Main model inputs, instrumental assumptions, and associated references. *Unless stated otherwise in the text.

Parameter	Value or/and reference
Stellar Input Spectra	F. Wunderlich et al. (2020) (see also Fig. 5)
Assumed distance of system	10 pc
LIFE Aperture, spectral range, [Resolution, $R = 100$]	Baseline Scenario* S. Quanz et al. (2022)
LIFE _{SIM} integration time, t	$t = 5$ and $t = 20$ d

the stellar spectra). Scenario 21 is as for scenario 20 (GJ832) but for AD Leonis (M3.V). Finally, scenario 22 is as for scenario 20 (GJ832) but for Proxima Centauri (M5.V). Table 1 shows the 22 scenarios performed. Note that all model parameters are as for the Earth Control (Scenario 1) unless otherwise stated. Table 2 shows the main inputs, assumptions, and associated references for the scenarios:

4. RESULTS

4.1 Atmospheric profiles

Fig. 1 shows 1D-TERRA model results for scenarios (1–8) (figure legend lower right).

In Fig. 1, temperature (K) (upper left panel) shows a ~ 20 K increase in the troposphere for the dark Earth (dark blue) scenario compared with the control scenario (blue), since the lowered surface albedo absorbs more incoming radiative energy, and a temperature decrease of similar magnitude for the bright Earth scenario. Results suggest a temperature increase of ~ 20 K in the middle to upper atmosphere for the scenarios with doubled and tripled gravity acceleration. This is associated with enhanced downward penetration of UV radiation due to the lowered atmospheric column. Regarding tropospheric water (H_2O) concentration (upper right), there were two main processes. First, changes in temperature, driving evaporation or condensation. For example, a warm troposphere, such as in the dark Earth resulted in a moist (~ 3 per cent vmr H_2O) surface. Secondly, changes in the user-input percentage relative humidity (per cent RH). For example, the dry Earth scenario (brown line) featured a decrease in tropospheric H_2O by over two orders of magnitude. Stratospheric H_2O varied from about 1 to 30 ppmv and changed proportionally more via upward mixing from the tropopause (in the lower stratosphere and for scenarios with weaker cold traps), and from methane (CH_4) oxidation in the middle to upper stratosphere, favoured by enhanced OH which increases with UV at higher altitudes. Regarding CH_4 , the dark Earth scenario (dark blue) features a warmer (hence wetter) troposphere, hence lies to the left of the light Earth scenario (light blue) due to more loss via OH. Water for the 3 g scenario increases strongly at the tropopause due to the switch from a fixed per cent RH (troposphere) governing the H_2O abundance, to instead strong chemical production of H_2O (from CH_4 oxidation) (stratosphere), which is stronger for the 3 g case (weaker column, stronger UV) than the 2 g case.

Regarding ozone (O_3) (lower left), results suggest rather small responses, related to established stabilizing feedbacks. For example, the changing gravity scenarios resulted in the O_3 peaks in the upper and middle stratosphere moving to lower altitudes due to the O_3 -UV feedback. Here, a decrease in the atmospheric column due to the gravity increase at constant surface pressure led to UV penetrating to greater atmospheric depths, enhancing O_2 photolysis on the lower levels, and resulting in the O_3 maximum moving downwards due to an enhanced Chapman cycle. CH_4 (lower right), responses ranged over about one order of magnitude and were mainly driven by UV and H_2O changes (see upper right). For the increased gravity cases, the smaller atmospheric column led to enhanced UV penetration and therefore to enhanced photolytic release of CH_4 sinks such as OH, Cl, and O^1D from their reservoirs. Nevertheless, the CH_4 concentration was larger than in the control. This arose because CH_4 surface emissions (constant in all scenarios) were released into

a smaller column domain of molecules for the increased gravity cases, which raised the CH_4 concentration (see also discussion in appendix). Fig. 2 is as for Fig. 1 but shows additional chemical profiles.

In Fig. 2, responses in nitrous oxide (N_2O) (upper left) were small, except for the two scenarios with increased gravity. Here, N_2O increased by up to an order of magnitude from the mid-stratosphere up to the mesosphere. This arose because (similar to the CH_4 response discussed above, see also discussion in Appendix) the constant surface flux of N_2O was released into a smaller column domain of molecules for the increased gravity cases, which raised the N_2O vmr. Note that there were no reductions in the main photochemical sinks for N_2O due to photolysis by UVB (see Fig. A1) or by reactions with electronically excited oxygen (O^1D) (see Fig. A2). Chloromethane (CH_3Cl) (upper right) responses were comparable to those of CH_4 (see Fig. 1), albeit somewhat larger; this is consistent with CH_3Cl having similar *in situ* sinks as CH_4 but being chemically more reactive due to its electronegative chlorine. HOx species (lower left) and NOx (lower right) are favoured mostly by stronger UV in the enhanced gravity scenarios (since the atmospheric column is smaller, see discussion above), which favours UV-release of HOx and NOx from important reservoirs such as H_2O and N_2O , respectively. NOx and HOx anticorrelate in the troposphere since they react with each other to form e.g. nitric acid (HNO_3); this phenomenon was discussed in B. Taysum et al. (2024). In addition to the above species, Figs A1–A3 in the appendix show UV profiles (A1), hydrogen-oxygen species (A2) and chlorine species (A3) for scenarios 1–8. Fig. 3 is as for Fig. 1 but shows scenarios 1 and 9–17 varying atmospheric mass and composition.

In Fig. 3 the temperature profiles (upper left) are broadly split into two groups. The first group of scenarios (blue shaded lines) have increasing surface pressure by adding N_2 as a fill gas (see Section 3, scenarios). In the upper and middle atmosphere, these profiles mostly overlie since they feature similar oxygen (hence ozone, lower left panel) amounts, which determine the temperature profile in this region. Surface temperature for this group remained approximately constant for the 2 and 5 bar scenarios compared with the control and decreased by a couple of degrees for the 10 bar scenario. This suggests that the transition from greenhouse warming into antigreenhouse cooling (since enhanced scattering leads to less net shortwave (SW) absorption) occurs at around 5 bar surface pressure. Note that enhanced N_2 leads to an increased efficiency of existing greenhouse gases due to enhanced gas-phase collisions. E. Keles et al. (2018) applied an earlier version of the model used here and suggested a similar result, namely that this transition occurs around 4 bar surface pressure for Earth-like (N_2 - O_2 dominated) atmospheres. To understand this issue further, Fig. A4 (see also Figs A5–A7) in the appendix shows radiative budget profiles for the scenarios shown in Fig. 3. The transition from greenhouse to antigreenhouse depends on the balance between total radiative heating (Fig. A4, centre lower panel) and total radiative cooling (right lower panel). Regarding the total heating, most scenarios (except the lower surface pressure scenario) overlap (i.e. different scenarios have similar total heating at a given pressure) in the middle and upper atmosphere, whereas in the lower atmosphere there are peaks that move to successively lower altitudes, diminishing in value with increasing pressure; these features form via a trade-off between incoming photons (abundant at high altitudes) and gas species (abundant at low altitudes). Peaks in the heating rate correspond to absorption of infrared, which re-emits and leads

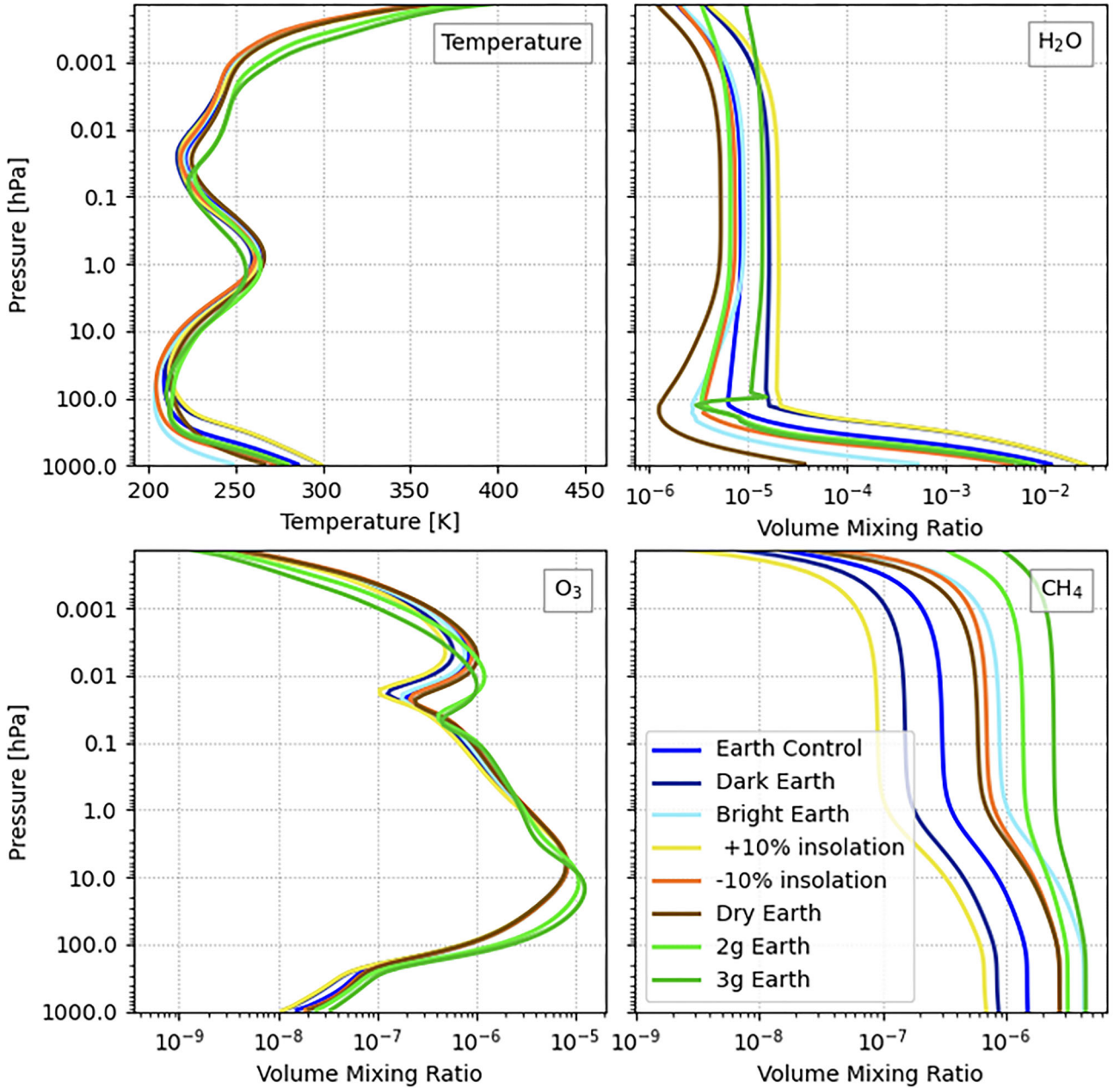


Figure 1. Global mean modelled atmospheric profiles of scenarios 1–8 (varying albedo, insolation, humidity, and gravitational acceleration) for temperature (K) (upper left), water (H_2O) (vmr) (upper right), ozone (O_3) (vmr) (lower left), and methane (CH_4) (vmr) (lower right) from 1D-TERRA.

to peaks in the total cooling rate (lower right panel) on similar pressure levels. The figure shows that thicker atmospheres scatter more SW radiation, which cools the lower regions. The second group of scenarios (grey shaded lines) in Fig. 3 show changing CO_2 abundances at constant surface pressure. Results suggest increasing surface temperature due to the enhanced CO_2 greenhouse effect, and a weakening in the tropopause temperature inversion, since O_2 (hence O_3) is lowered in abundance being replaced with CO_2 .

Water abundances in Fig. 3 (upper right) increase with temperature due to strengthened evaporation in the troposphere; in addition, water reaches large abundances above the tropopause for scenarios with weakened temperature inversions (hence weaker upward mixing). O_2 and O_3 in the 90 per cent CO_2

scenario are produced primarily via photolysis of CO_2 , which forms $\text{CO} + \text{O}$, followed by the O-atom self-reacting to form O_2 . Finally, this O_2 forms O_3 by reacting with atomic oxygen. O_3 in Fig. 3 (lower left) is reduced by only around a factor of 2 to 3 for most scenarios in the middle atmosphere (despite increasing H_2O , hence more HOx, a sink for O_3). This behaviour is consistent with the well-established negative O_3 -UV feedback (here, e.g. less O_3 leads to more UV penetration, hence more O_2 photolysis which stabilizes O_3 abundances; T. Kozakis et al., 2022). This mechanism can help to maintain O_3 abundances over widely differing conditions. Regarding CH_4 (lower right), for the N_2 - O_2 scenarios (blue lines), going from 2 to 5 to 10 bars surface pressure, CH_4 decreased due to the higher number density of OH, the main CH_4 sink (despite a cooler drier atmosphere, which,

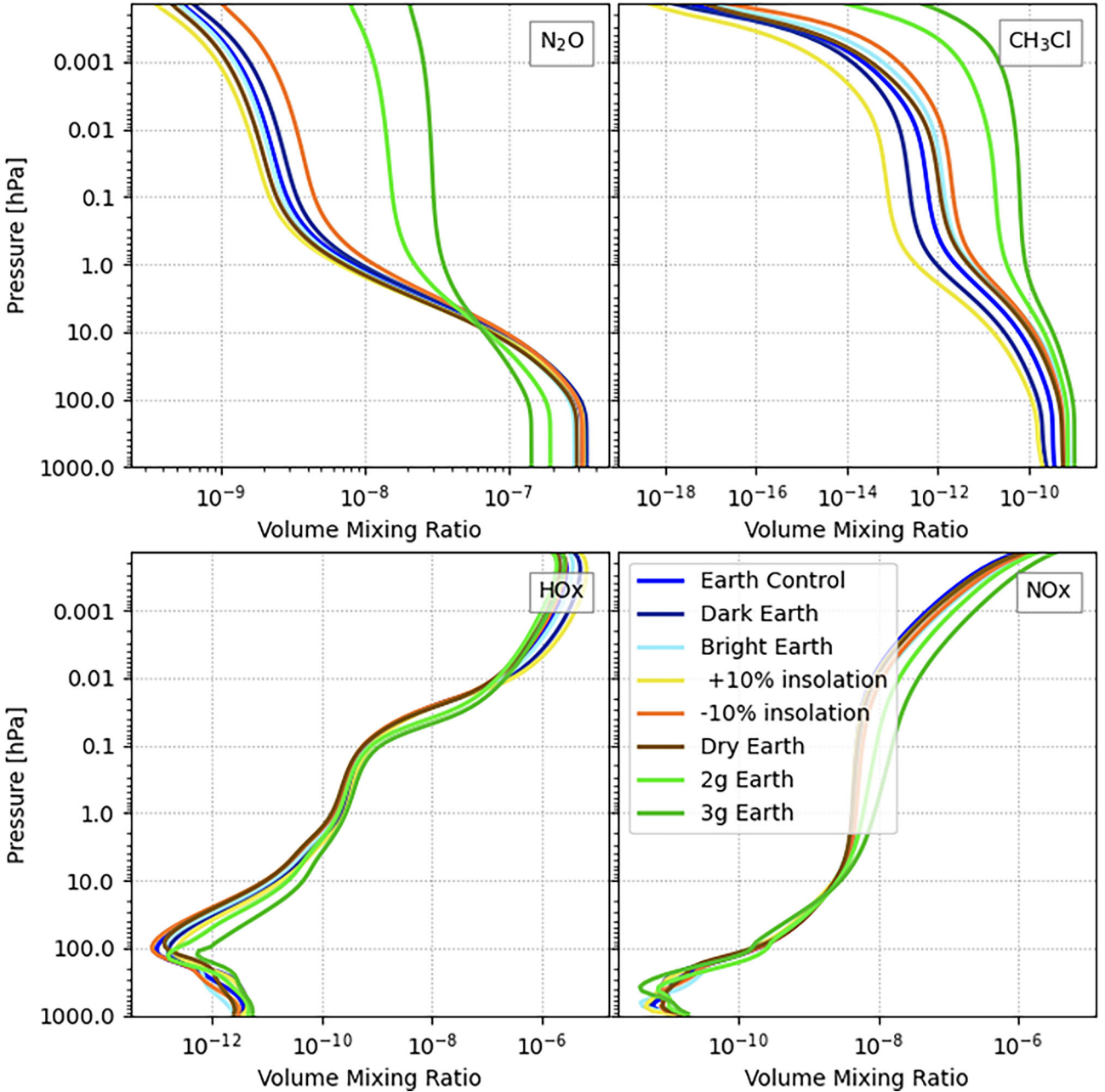


Figure 2. As for Fig. 1 but showing N_2O (upper left), CH_3Cl (upper right), HOx ($=\text{H} + \text{OH} + \text{HO}_2$) (lower left), and NOx ($=\text{N} + \text{NO} + \text{NO}_2 + \text{NO}_3$) (lower right).

all else being equal, would tend to reduce OH). Secondly, for the scenarios with CO_2 increasing from 10 to 90 per cent (at 1 bar surface pressure, grey lines), CH_4 increases; this occurred despite warming due to the stronger CO_2 greenhouse, which leads to evaporation and would in this sense favour more OH hence less CH_4 . Inspecting the OH profile (Fig. A6, upper left panel), however, suggests the response to changing CO_2 is not straightforward and differs with altitude. Increasing CO_2 increases absorption for $\lambda > \sim 150$ nm in the middle to upper atmosphere and can lead to complex responses in O_3 (with its altitude-dependent catalytic chemistry) and UV, which influence OH via its main source reaction: O^1D (mainly from O_3 photolysis) + $\text{H}_2\text{O} \rightarrow 2\text{OH}$.

Figs A5–A7 show UV profiles (A5), hydrogen-oxygen species (A6), and chlorine species (A7) for scenarios 1 and 9 to 17. It is notable that, for the scenario with 10 times reduced atmospheric mass (surface pressure, $P_0 = 100$ mb), active chlorine species (Cl and ClO) (efficient in destroying O_3 in the upper stratosphere) are strongly enhanced by two to three orders of magnitude from the tropopause upwards. This arose first because the biomass surface fluxes of the chlorine-containing reservoir chloromethane were kept constant for all scenarios, which leads to a stronger vmr of total chlorine on reducing the overall atmospheric mass by $\times 10$. Secondly, an important form of chlorine in Earth’s upper stratosphere and mesosphere is the reservoir, hydrochloric acid (HCl). This strongly bound molecule is photolysed below ~ 220 nm in

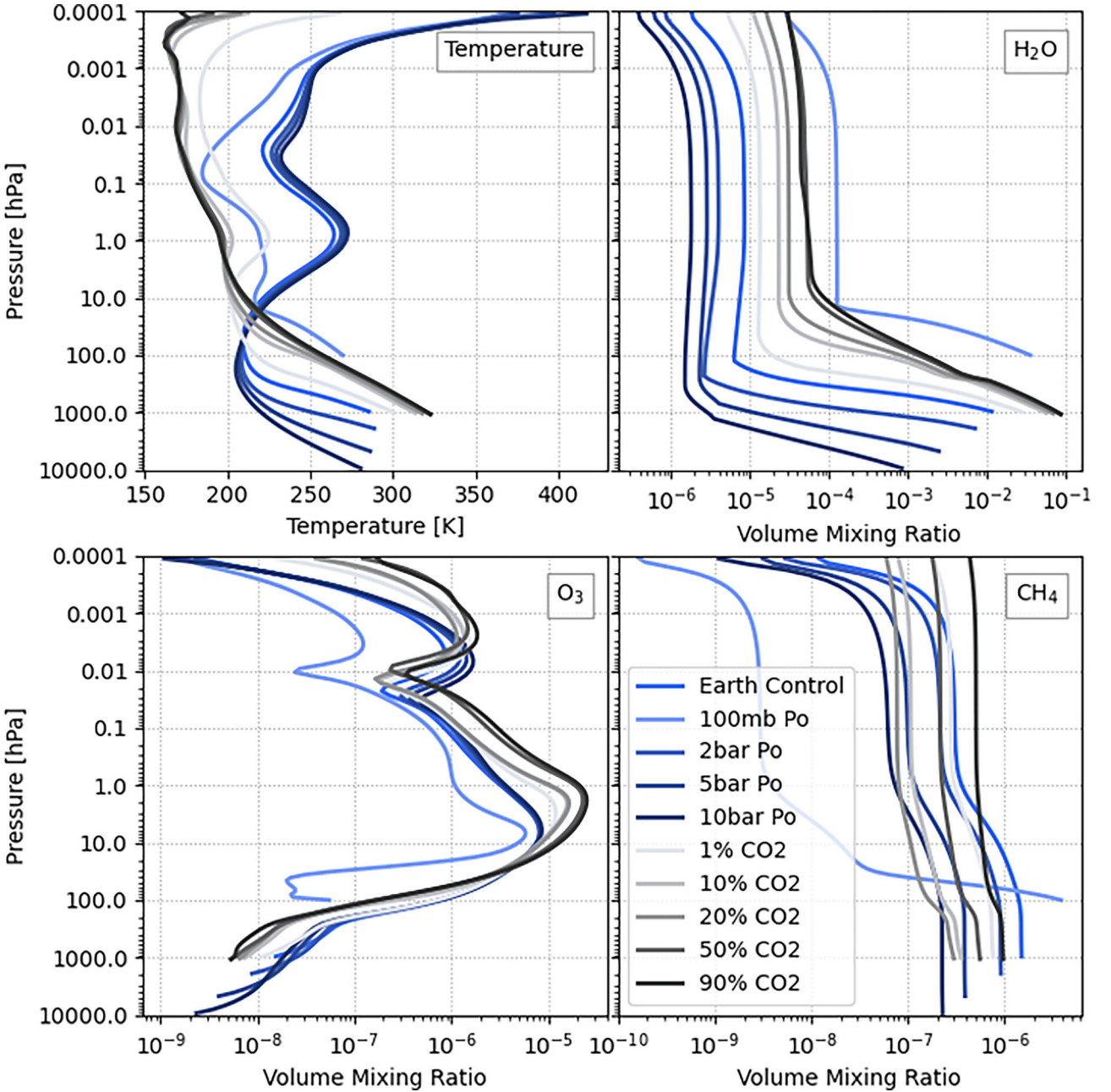


Figure 3. As for Fig. 1 but for scenarios 1 and 9–17 (varying atmospheric pressure and composition). For orientation, the grey lines with tones increasing from light to dark grey denote increasing CO₂ and they generally increase monotonically in tone from left to right in each of the upper two panels. Similarly, the blue tones become darker in hue with increasing pressure; for orientation the blue tones can be distinguished by inspecting the pressure jumps in the surface values in the temperature panel (upper left) or/and the water panel (upper right) where warmer temperatures (lighter blue) lead to wetter atmospheres.

the UVC (see e.g. M. Bahou et al., 2001), where UVC is defined as follows: $175.0 \text{ nm} < \lambda < 281.1 \text{ nm}$. UVC is strongly enhanced for the scenario with x10 reduced atmospheric mass (Fig. A5) in the middle atmosphere. Fig. 4 is as for Fig. 3 but shows N₂O, CH₃Cl, HOx, and NOx.

Fig. 4 suggests increased abundances of both N₂O (upper panel left) and CH₃Cl (upper panel right) in the mid to upper atmosphere for the enhanced CO₂ scenarios (grey lines). This was mainly due to atmospheric shielding by CO₂ which slowed their photolytic destruction rates. HOx and NOx (lower panels in Fig. 4) were modestly increased (especially so for NOx) for

the enhanced CO₂ scenarios, especially in the upper levels. Here, despite the increased shielding effect (which by itself would favour a decrease of HOx and NOx due to weakened photolytic release from their reservoirs), the HOx and NOx increase seen in Fig. 4 (grey lines in the upper atmosphere) was favoured e.g. by enhanced O¹D (from CO₂ photolysis) which led to release of HOx (e.g. via: O¹D + H₂O → 2OH) and NOx (e.g. via: O¹D + N₂O → 2NO). Fig. 5 shows the stellar spectra used for scenarios 1 and 20 to 22 (see F. Wunderlich et al., 2020 for more details).

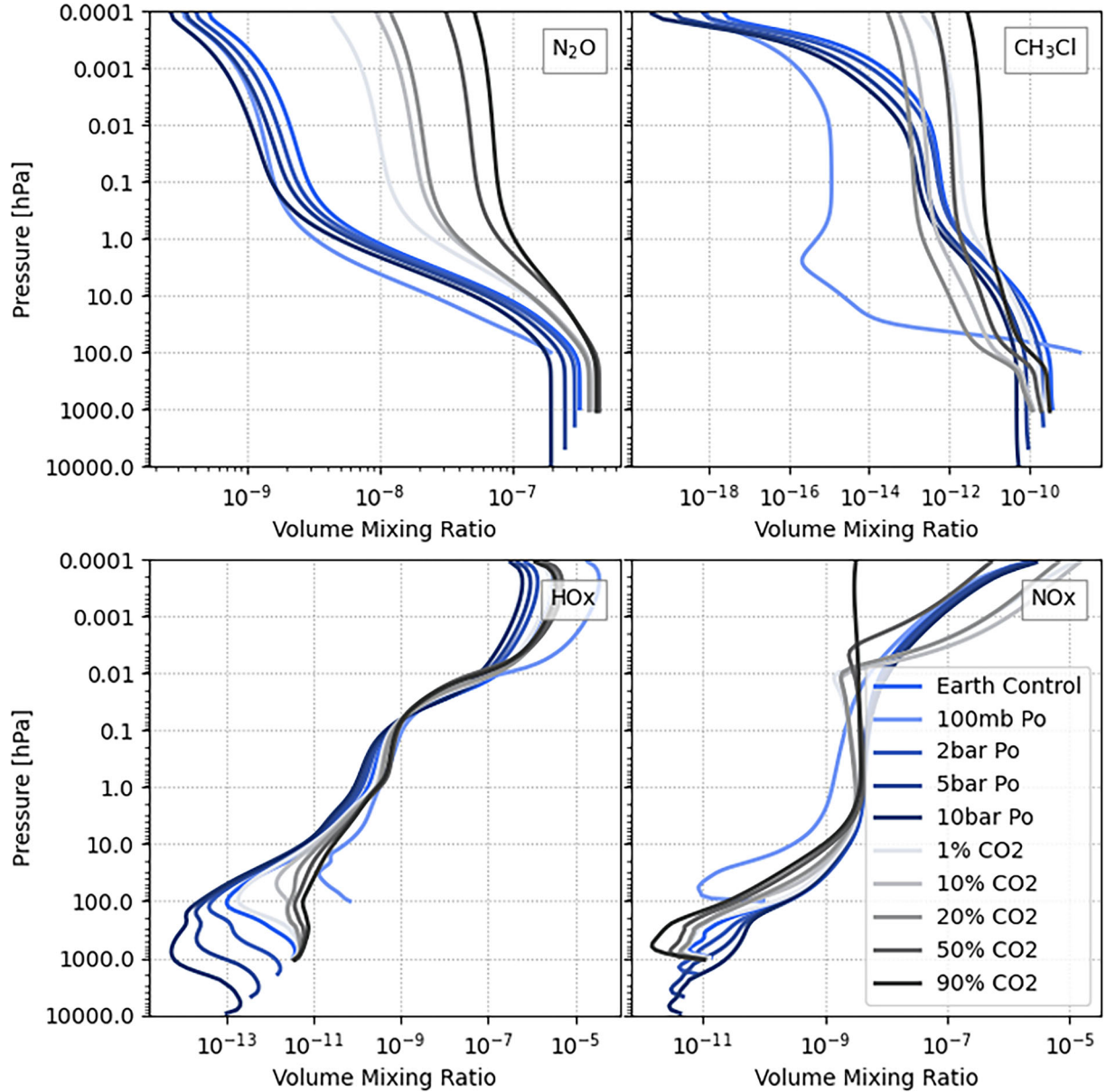


Figure 4. As for Fig. 3 but showing N_2O (upper left), CH_3Cl (upper right), HOx ($=\text{H} + \text{OH} + \text{HO}_2$) (lower left), and NOx ($=\text{N} + \text{NO} + \text{NO}_2 + \text{NO}_3$) (lower right).

Fig. 6 is as for Fig. 1 but shows scenarios 1 and 18–22, which involve varying the incoming stellar spectrum and the eon (Archaean and Proterozoic instead of modern Earth) (see Table 1). Note that the Archaean extends from about 4 to 2.5 Gyr ago, whereas the Proterozoic extends from about 2.5 to 0.5 Gyr ago.

In Fig. 6, temperature profiles (upper left) for the three scenarios simulating planets orbiting cool central stars suggest surface temperatures increasing from 288 K (control) to ~ 300 K. This is mainly due to greenhouse heating from enhanced ($\sim \times 100$ compared with the control) CH_4 abundances (lower right panel), which arose because weaker UVB emission from the cooler stars led to a reduction in atmospheric planetary OH, an important CH_4 sink. This effect is well established (see e.g. A. Segura et al., 2005; J. L. Grenfell et al., 2007; S. Rugheimer et al., 2015). In the upper atmosphere, the three scenarios with cooler central stars featured strong reductions in CH_4 and H_2O (its photolytic

product), related to the enhanced stellar UVC sinks. Temperature profiles also lacked the stratospheric inversion feature for all scenarios except the Earth control. This arose due to weaker O_3 heating, either due to a reduction in incoming stellar UV or/and via weaker Chapman production of O_3 (lower left) via O_2 photolysis. Despite strongly reduced O_2 in the Proterozoic and Archaean scenarios, O_3 abundances were reasonably stable, due to the O_3 -UV photochemical feedback (see e.g. A. Segura et al., 2003). Water profiles (upper right) were mostly dependent on temperature, whereby tropospheric warming favoured damper atmospheres via evaporation. Regarding the Archaean and Proterozoic scenarios, an important effect was enhanced UV penetration due to the reduction in O_2 hence O_3 . This in turn led to increased OH (which is photolytically produced) and therefore to a reduction in CH_4 and its photolytic

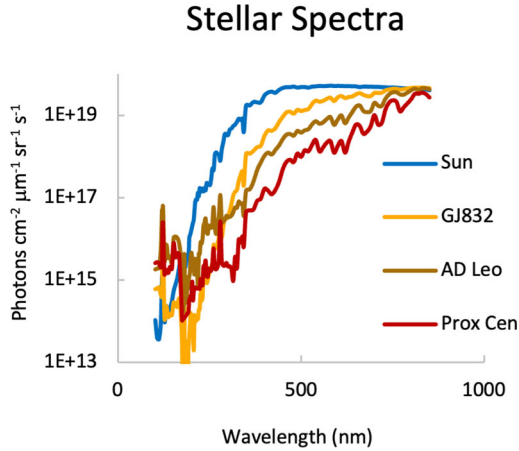


Figure 5. Incoming stellar spectra for scenario 1 (Sun, blue); scenario 20 (GJ832, orange); scenario 21 (AD Leo, brown), and scenario 22 (Proxima Centauri, red).

product, H_2O . Fig. 7 is as for Fig. 6 but for differing chemical species.

In Fig. 7, the potential biosignature, nitrous oxide (N_2O) (upper left), is enhanced for the cool star scenarios since stellar UVB emission (a photolytic sink for N_2O) is weaker. On the other hand, N_2O is decreased for the Proterozoic and Archaean scenarios, since UVB abundances are stronger compared with the control scenario, due to the reduced O_3 layer for these reduced O_2 atmospheres. Chloromethane (upper right) has similar chemical sinks as CH_4 (Fig. 6) and therefore broadly similar responses. Figs A8–A10 show UV profiles (A8), hydrogen-oxygen species (A9), and chlorine species (A10) for scenarios 1 and 18–22; results suggest that the effect of changing the central star has a strong effect upon atmospheric UV profiles as well as the HOx and ClOx families and reservoir chemistry in Earth-like (N_2 – O_2 dominated) atmospheres.

4.2. Spectral radiance

Fig. 8 shows theoretical emission spectra with a spectral resolution, $R (= \lambda/d\lambda) = 100$, calculated by the GARLIC model based on (T, p, composition) input profiles from 1D-TERRA for the same three groups of scenarios as shown in Section 4.1.

In Fig. 8 the upper panel indicates spectral features due to H_2O and CH_4 in the IR at ~ 6 microns (for the dry Earth scenario the H_2O band is weakened), a persistent O_3 band at ~ 9.6 microns and the CO_2 main band at ~ 15 microns. In the middle panel, again apparent are the H_2O and CH_4 bands at ~ 6 microns, as well as the O_3 band at ~ 9.6 microns; the CO_2 fundamental for the low-mass atmosphere ($P_0 = 100\text{mb}$, orange line) scenario is considerably weakened, related to the cooler middle atmosphere temperatures via reduced O_3 (see Fig. 3). In the lower panel, the O_3 9.6 microns feature is reduced due to reduced UVB from the star, leading to weakened Chapman production. The CO_2 band at ~ 15 microns is rather deep for the Proterozoic and Archaean scenarios which featured reduced O_2 hence cooling in the upper layers. Fig. 9 shows a matrix plot summarizing absolute differences in the emission spectra shown in Fig. 8 for the 22 scenarios.

Fig. 9 consists of a matrix which summarizes the mean, absolute differences in the planetary spectral radiance ($\text{W m}^{-2} \text{sr}^{-1} \text{micron}^{-1}$) for all 22 model scenarios, $\Delta_{ij} = \text{mean}(|I_i - I_j|)$ where $i, j = 1, \dots, 22$ and I_i denotes the emission spectrum of scenario,

i. The figure shows results for two central emission bands in Earth-like atmospheres: first, the CO_2 15 μm band (upper right triangle) and second, the O_3 9.6 μm fundamental band (lower left triangle). How these two bands are treated is illustrated in the Appendix, Fig. A12.

Regarding the CO_2 band (upper right triangle) largest differences occur in two regions, marked with the red and green boxes. The row of red boxes suggests that starting with low-pressure ($p_0 \sim 100\text{mb}$) atmospheres (scenario 9), emission is particularly sensitive to changes in atmospheric mass and composition (scenarios 10 to 19). The green boxes suggest that scenarios with cooler central stars (scenarios 20–22) are particularly sensitive to changing CO_2 concentration (scenarios 14 to 17). [Note however there is a caveat here – the differences shown depend not only on changes in the atmosphere, but also changes in the stellar spectra]. In general, the strong CO_2 molecule is chemically rather unreactive and its absorption band responds more sensitively to temperature differences rather than chemical changes, as denoted by the red and green boxes.

Regarding the O_3 band (lower right triangle in Fig. 9) largest differences occur in two regions, marked with the yellow and orange boxes. The yellow boxes suggest that the bright Earth scenario (scenario 3) responds sensitively to changes in atmospheric mass, composition, eon, and (especially) central star. The row of orange boxes suggests that the scenarios with cooler central stars (scenarios 20–22) respond sensitively to the UV environment and atmospheric mass (scenarios 3–12). In general, the O_3 molecule is chemically reactive and its absorption band responds more sensitively to the availability of UV which drives photochemical responses in Earth-like atmospheres. Although not the main focus for LIFE, for completion we show transmission spectra in the appendix Fig. A11.

4.3 Detectability using LIFE_{SIM}

Fig. 10 shows the spectral detectability with LIFE_{SIM} of five key atmospheric species using the baseline instrument scenario (S. Quanz et al., 2022) for targets at 10 pc assuming 5 d (light shading) and 20 d (dark shading) viewing times. Note that each sub-panel compares two scenarios; these were chosen because they cover the full range from a weak to a strong species' signal after inspecting all scenarios:

In Fig. 10, a central aim is to determine to what extent a given species' band stands out from the noise. Each panel in Fig. 10 is centred on the wavelength of a strong spectral feature for the particular species indicated. For example, for O_3 , the weak scenario is taken to be the Proterozoic scenario (with reduced O_2 hence weakened O_3), whereas the strong scenario is the modern Earth with its thick O_3 layer. We adopted the format of Fig. 10 since in our previous detectability papers (e.g. F. Wunderlich et al., 2020) we assumed that detectable features occur where data points are able to resolve spectral features which lie outside the shaded (instrument noise) region; their procedure can be conceived as follows. Centred at the Planck curve, we depict the wavelength-dependent noise as a shaded region. We then add the spectral bands based on a single (global mean) calculation of spectral absorption features from the theoretical spectral model (GARLIC, see Section 2.3) based on input from our atmospheric climate-chemistry model (1D-TERRA, see Section 2.2). We also perform retrieval studies (see below) in order to calculate the

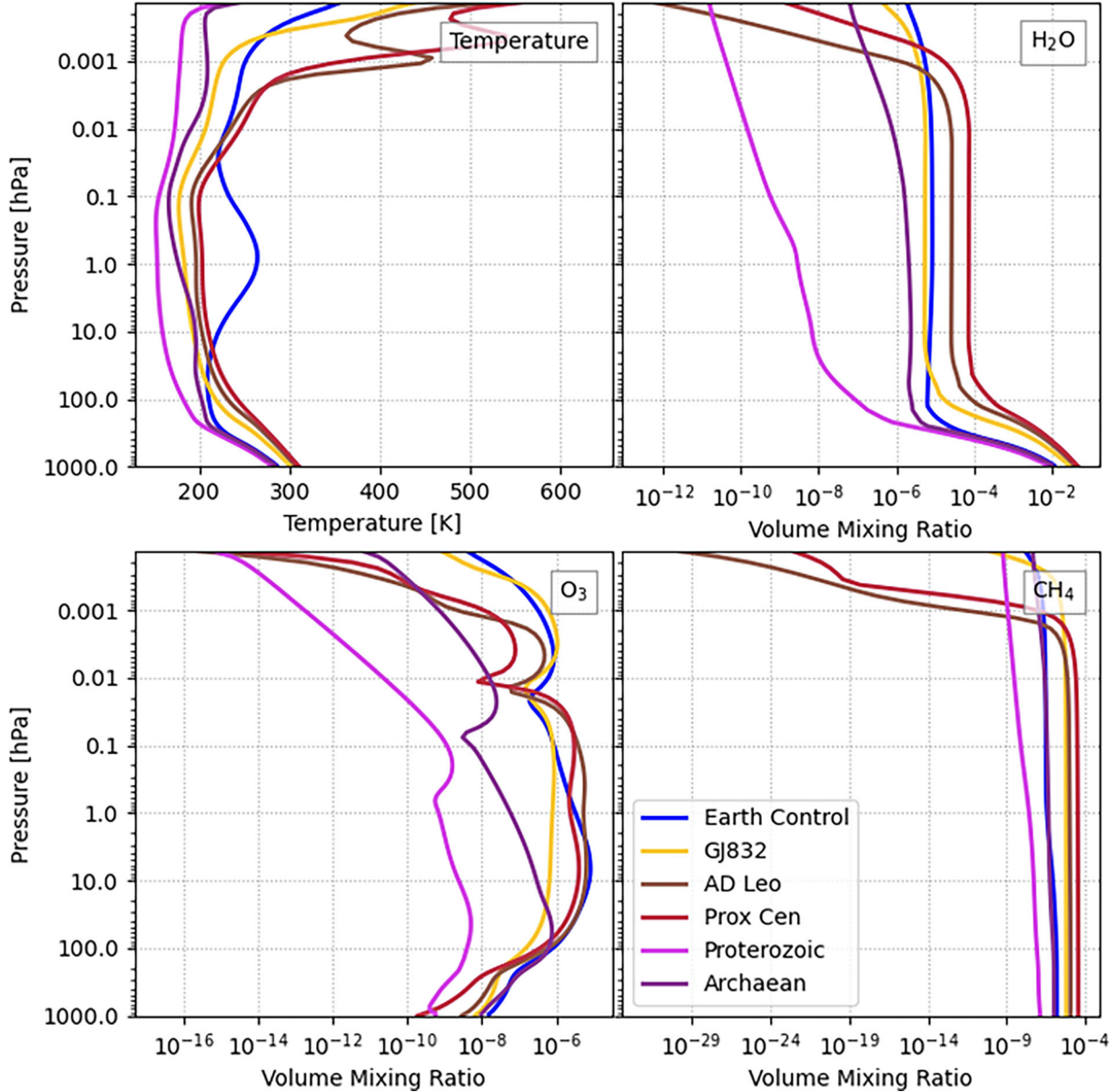


Figure 6. As for Fig. 1 but for scenarios 1 and 18–22 varying the top-of-atmosphere stellar spectrum and the eon (Archaean and Proterozoic).

significance of detection for a given species. Note that Fig. 10 does not show CH₄ (e.g. for the rotational–vibrational hot bands in the near-IR) because of the high photon noise at these wavelengths. CH₄, however, is still retrievable for some scenarios due to band absorptions at longer wavelengths (see Section 4.4).

Panel (a) (H₂O) in Fig. 10 suggests weak signals with strong scatter for the dry and wet scenarios considered. This arises mainly because the emission spectra of habitable planets are dominated by strong photon-noise in this wavelength region (see e.g. F. A. Dannert et al., 2022). Panel (b) (HNO₃) also suggests rather weak signals and strong scatter for both considered scenarios. Panel (c) (N₂O) suggests lowered noise (mainly associated with enhanced photon emission at these higher wavelengths) compared to the two previous cases, with an indication that the data points are able to resolve the N₂O absorption band at around 7.8 microns, especially for the high N₂O scenario (‘Earth’ orbiting Proxima Centauri) (purple dots). Data points in panel (d) (O₃) indicate a discernable minimum corresponding to the O₃ funda-

mental band at around 9.5 to 9.6 microns, especially for the thick O₃ layer of the Earth control scenario. The strong CO₂ spectral feature at around 15 microns in panel (e) is not only discernible for both scenarios, but results also suggest that the two scenarios are distinguishable (no overlap of shaded regions).

4.4 Atmospheric retrieval

4.4.1 Estimate of surface temperature

Fig. 11 shows emission spectra calculated with GARLIC (black line, $R = 100$) for the Earth control scenario with a viewing time noise calculated for 5 d (panel 11a) and 20 d (panel 11b), the Proterozoic scenario (panel 11c), and the Earth around Proxima Centauri scenario (panel 11d). Also depicted are Planck curves (solid red line) for the temperatures (solid red line) and temperature ranges (dotted and dashed red lines) shown.

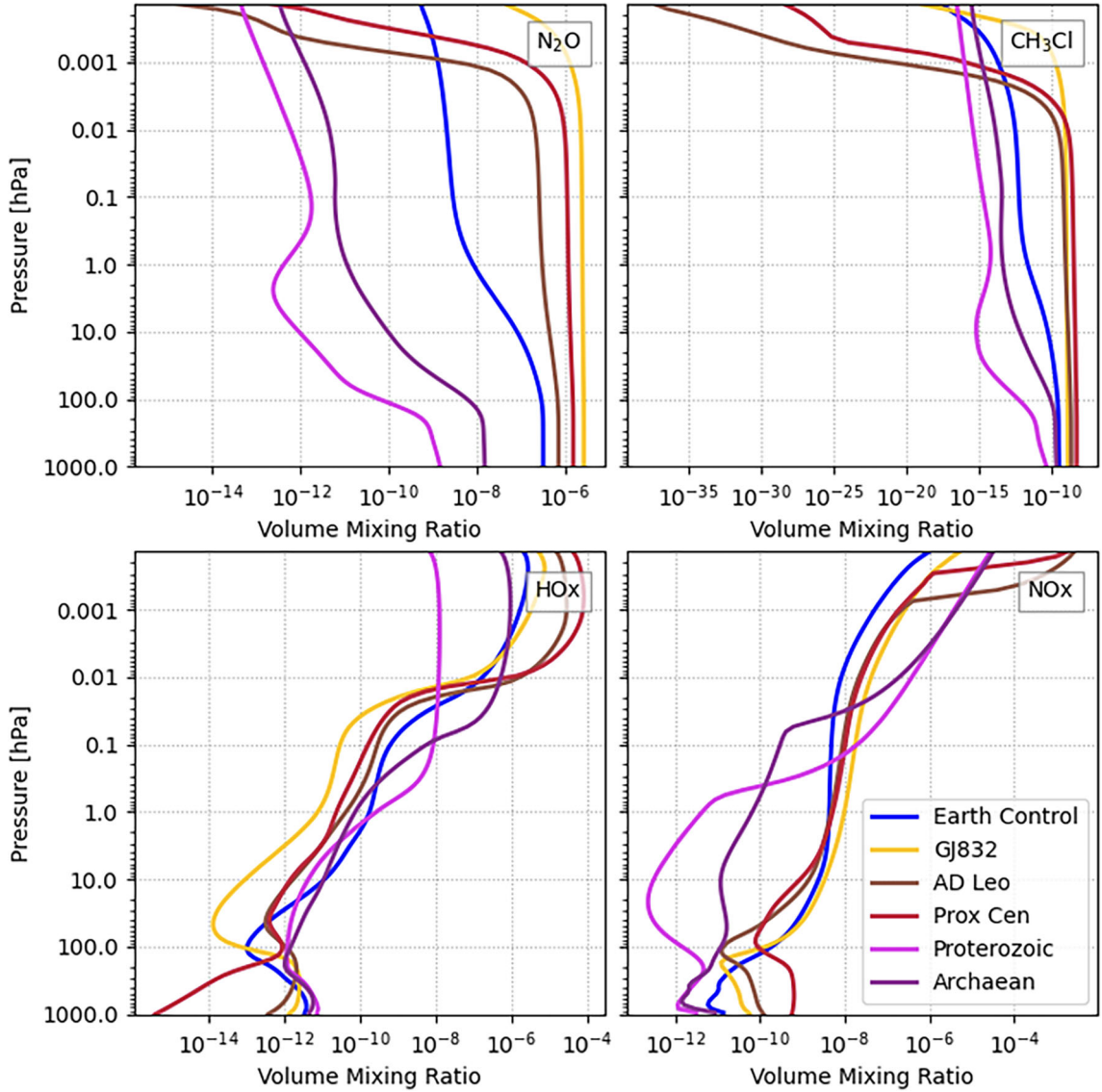


Figure 7. As for Fig. 6 but showing N_2O (upper left), CH_3Cl (upper right), HOx ($=\text{H} + \text{OH} + \text{HO}_2$) (lower left), and NOx ($=\text{N} + \text{NO} + \text{NO}_2 + \text{NO}_3$) (lower right).

In Fig. 11, starting with Garlic emission spectra, we first add noise. This can lead to negative values especially in lower wavelengths. The figure shows the absolute values with added noise, which is different for the 5 d and 20 d cases. Fig. 11(a) suggests that a 5 d short-viewing would suffice to obtain a first estimate (± 50 K) of the sampled temperature in the emitting layer. This information would provide important constraints as to whether the planet features an atmosphere. Then, if required, the longer, 20 d viewing (Fig. 11b) could be applied for a more accurate (± 10 K) determination. The scenarios shown in Fig. 11 were chosen to represent a reasonable range of temperature from all scenarios. Further inferring the planet's surface temperature hence its potential habitability, however, would require additional information, including atmospheric composition, as reviewed in e.g. L. Kaltenegger (2017).

4.4.2 Column retrieval: composition

Figs 12(a)–(h) show results from the atmospheric column retrieval algorithm (Section 2.5) for five trace gases ($R = 50$) with significances larger than 1 – shown here for the LIFE *optimistic* instrument set-up (S. Quanz et al., 2022). Note that the strong increase in photon noise (see previous section) at wavelengths smaller than $\sim 8 \mu\text{m}$ inhibits a robust retrieval of signals in this wavelength range; this affects mainly water vapour retrieval. Methane (CH_4) and nitrous oxide (N_2O) have overlapping bands, inhibiting the retrieval of the narrower N_2O signal, and reducing the significance of the CH_4 signal.

Table 3 shows the detectability confidence level (in sigma) of scenarios (chosen to have $\sigma > 1$ for most of the key species shown) calculated by the KIT retrieval model performed for the *optimistic* aperture and baseline (S. Quanz et al., 2022), a spectral resolution ($R = 100$) and a 20 d integration time for a spectral range of 4 to 18 microns.

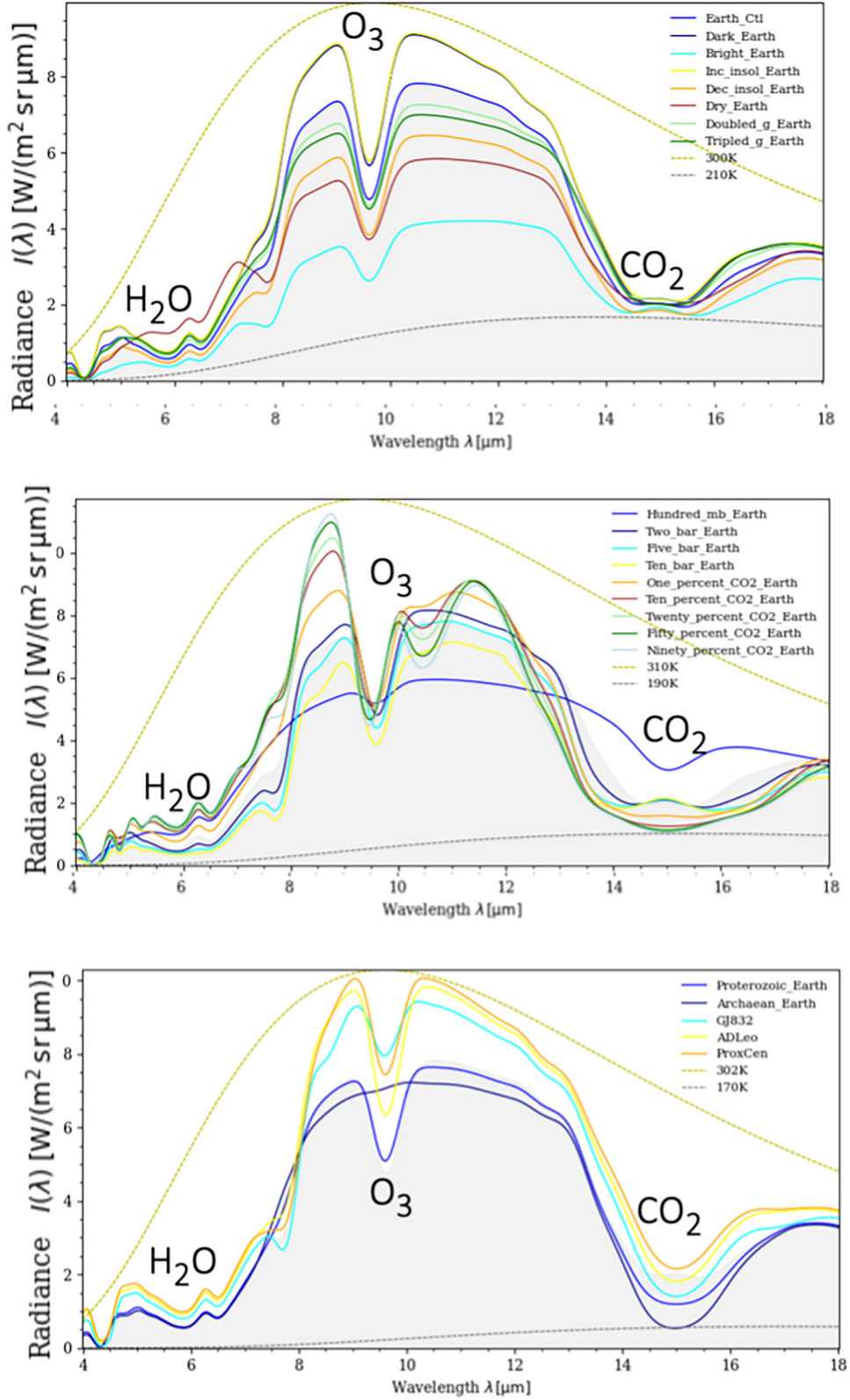


Figure 8. Theoretical IR emission spectra ($R = 100$) calculated by GARLIC for scenarios 1–8 (varying albedo, orbit, and gravity) (upper panel); scenarios 1 and 9–17 (varying atmospheric mass and composition) (middle panel) and scenarios 1 and 18–22 (varying photon flux from central star and eon) (lower panel). The grey shading shows modern Earth radiance. The dashed lines show the corresponding Planck curve temperature as indicated in the legend.

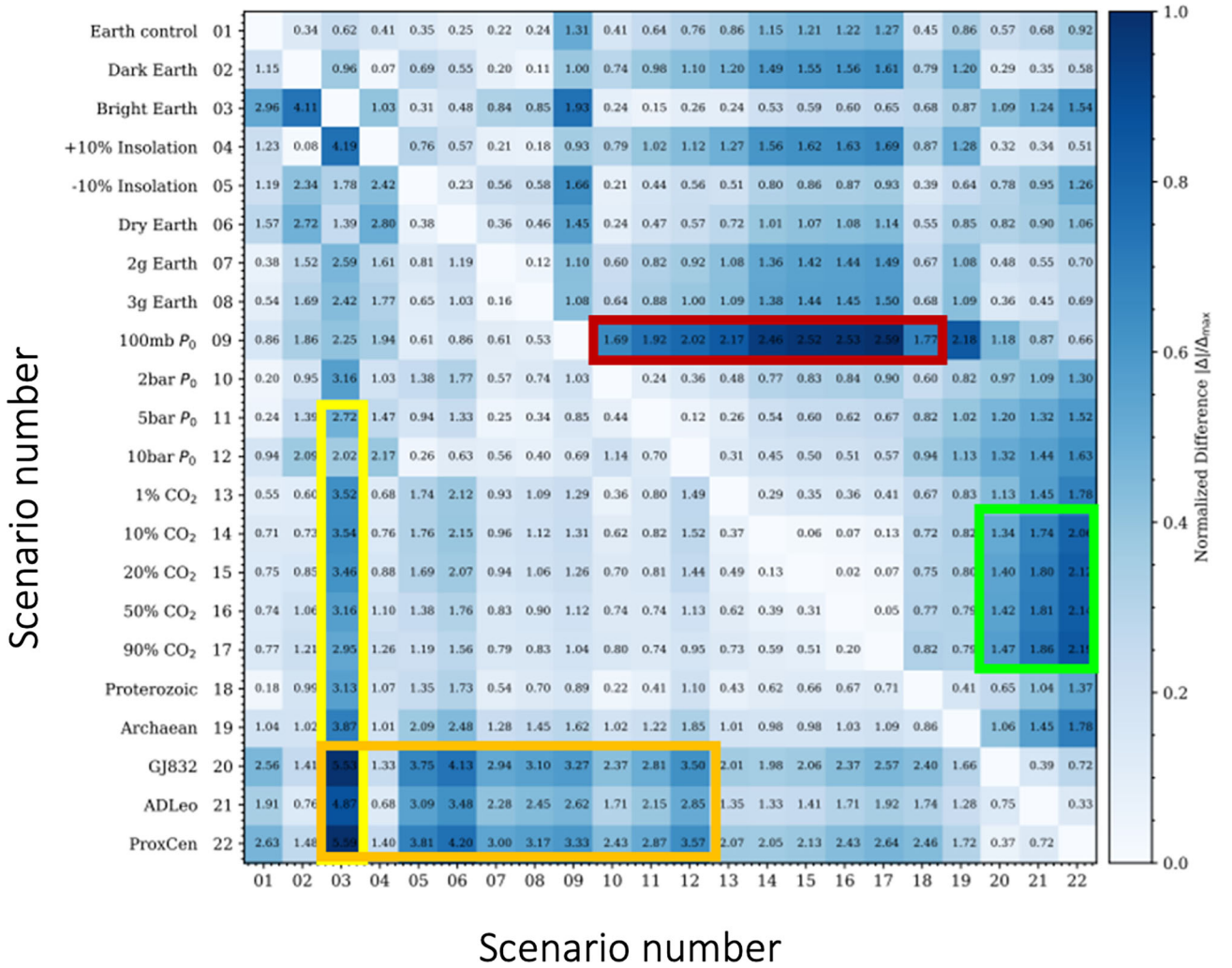


Figure 9. Matrix plot summarizing the main differences between the 22 model scenarios. The x- and y-axes show the scenario numbers. The values in the blue-shaded boxes show the absolute mean difference (Δ) of the spectral radiance ($\text{W m}^{-2} \text{sr}^{-1} \mu\text{m}^{-1}$) taken from the calculated emission spectra (Fig. 8). The darker blue shading corresponds to larger Δ values. The upper right triangle (above the central diagonal, denoted by empty white boxes) shows Δ values for the CO_2 fundamental absorption band at 15 microns. The lower left triangle shows the same but for the O_3 fundamental absorption band at 9.6 microns. The coloured boxes (red, yellow, green, orange) represent large emission differences (deeper blue shading).

Results in Table 3 can be summarized as follows. Water is challenging to retrieve in most scenarios, since many of its spectral bands occur in the near-IR, where the instrument is photon-starved hence features high noise (an Earth-like planet emits only weakly in this region, see e.g. Planck curve in Fig. 8 at ~ 4 microns); water retrieval is somewhat favoured for the ProxCen scenario since the atmosphere is rather wet due to surface greenhouse warming, which leads to some ocean evaporation. Nitric acid is also generally difficult to retrieve in most scenarios. N_2O is not retrieved to a confidence level of greater than 0.7σ . Ozone by comparison is generally well retrieved, except for e.g. the Archaean and 100mb scenarios which features low oxygen (hence low ozone) abundance. CO_2 is generally challenging to retrieve for opaque atmospheres such as the thick 90 per cent CO_2 scenario. J.-N. Mettler et al. (2024) investigated (p-T) retrieval of Earth-like planets 10 pc away using LIFE and found that temperature profiles could be constrained to within a few tens of K.

4.4.3 Profile retrieval: temperature

Fig. 13 shows temperature profiles from a selection of representative scenarios retrieved from (synthetic) long-wave IR thermal emission spectra comprising the strong CO_2 band around $15 \mu\text{m}$. Two sets of retrievals have been performed, for low and moderate resolution [half width 7.0 and 0.7 cm^{-1} with resolutions R of approximately $R = 100$ (corresponding to the LIFE baseline) and $R \sim 1000$, respectively]. Molecular concentrations and the initial guess temperature are taken from models of Earth's tropical, mid-latitude summer/winter, and subarctic summer/winter atmospheres. Figs 13(a)–(h) show results from the atmospheric profile retrieval algorithm for temperature (Section 2.6) for eight model scenarios (Table 1), which give a representative range of temperature.

Results in Fig. 13 suggest that for all atmospheres, temperature can be estimated quite well for low altitudes up to about 20 km (for the Proxima Centauri scenario the deviation is somewhat

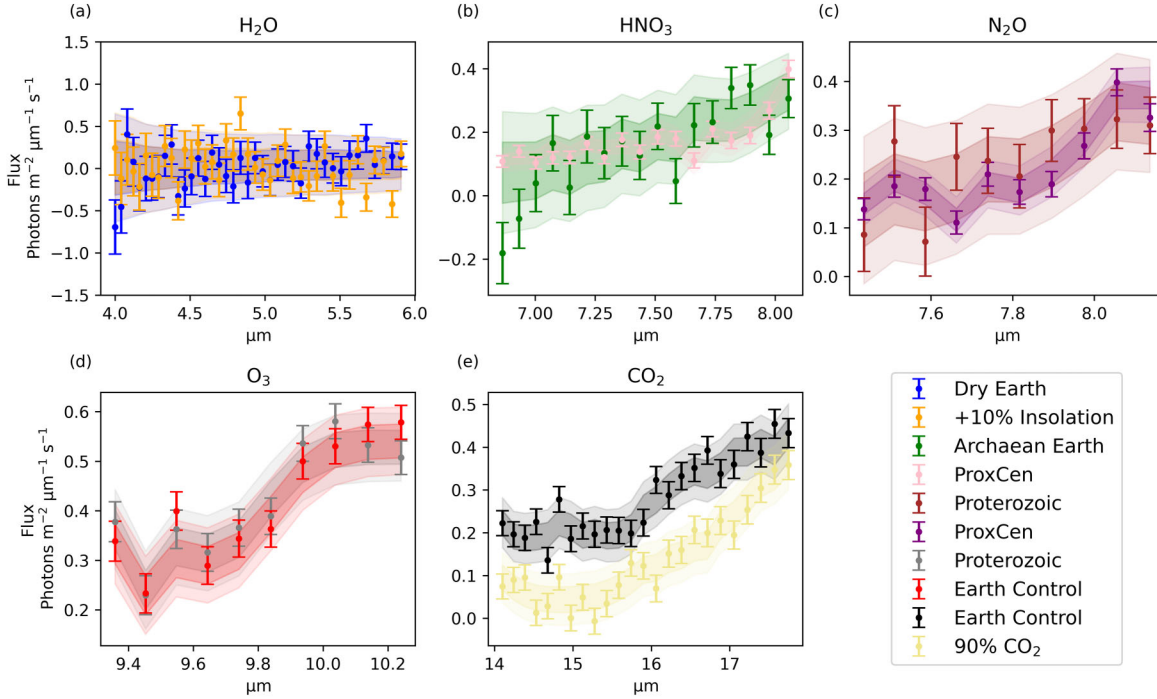


Figure 10. Detectability of five key atmospheric species estimated with LIFE_{SIM} assuming a target at 10 pc for 5 d (light shading $\pm 1\sigma$) and 20 d (dark shading $\pm 1\sigma$) integration time. The error bars shown indicate results for the 20-d integration. LIFE_{SIM} was run with wavelength resolution, $R (= \lambda/d\lambda) = 100$. Panels originally using the same scenario colours as in previous figures was rejected since this produced shading overlap colours, which led to difficulties in distinguishing the scenarios. Each panel shows two chosen scenarios, which cover the full range (from weak to strong spectral features) where text in the legend indicates the model scenarios shown in Table 1.

larger). In the middle atmosphere discrepancies between true and retrieved temperatures become evident especially for the low-resolution runs. Above about 50 km, the low-resolution spectra provide virtually no information on temperature, whereas the moderate resolution performs somewhat better. This is in accordance with the Jacobian and weighting functions discussed in the SVEETIES study (F. Schreier et al., 2020), i.e. at reduced resolution the sensitivity to higher altitudes is decreased.

5. DISCUSSION

A unique contribution of this work is that we perform consistent end-to-end calculations with dataflow from climate-chemistry model to theoretical spectral model to noise simulation tool. How robust are our results? One of the main uncertainties is the assumption of an Earth-like bulk atmosphere (N_2 - O_2 dominated). Given this assumption, chemical networks applied in the literature predict generally similar responses. Moving however to atmospheres not similar to Earth i.e. dominated by e.g. CO_2 , H_2O , or H_2 from Mars-like to Venus-like (p, T) conditions then it is less clear whether available chemical schemes would produce generally similar responses – here more data are needed e.g. for biosignature reactions in different bathgases, over a suitable range of (T, p), etc.

To what extent do the different scenarios here cover more generally the variation of parameters in reality? The scenarios cover a good range based on what we know of the modern Solar system, the Early Earth, and stellar spectra. For the scenarios in this work, surface biomass fluxes are mostly based on the modern Earth (F. Wunderlich et al., 2020). Exceptions to this were the 90 per cent CO_2 run and the Archaean run, which used mid Archaean

$O_2 = 10^{-5}$ vmr, and the Proterozoic run, which used O_2 reduced by $\times 100$ compared to the modern Earth based on discussions in e.g. D. C. Catling and M. W. Claire (2005). The appropriateness of applying modern Earth biomass fluxes to our scenarios is difficult to assess since knowledge on how (or if) life would evolve on Earth-like planets is not well constrained. Changing atmospheric properties will impact surface life evolution by changing UV exposure. Life requires some minimum UV exposure to drive evolution, but too much UV is deadly. The range of surface UV needed to drive evolution is however not well constrained.

If the Solar system is not typical then our chosen range may not include effects such as exoplanets experiencing e.g. HEP bombardment, high eccentricity, etc. Recent studies have investigated such effects. For example, R. J. Ridgeway et al. (2025) and K. Herbst et al. (2024) investigated the effect of HEPs in rocky exoplanetary atmospheres with a 3D and 1D model suite, respectively. M. J. Way et al. (2023) modelled the effect of varying eccentricity upon the climate of an Earth-like planet.

Regarding 3D model studies of Earth-like planets, atmospheric climate and composition depend on various factors, such as the land-sea distribution and the atmospheric circulation, which are not constrained for Earth-like planets. Regarding atmospheric biosignatures, there is an important feedback between atmospheric ozone heating and transport, where stronger ozone heating at low latitudes increases the latitudinal temperature gradient hence strengthens the meridional circulation. On tidally locked Earth-like planets, this feedback can affect the strength and shape of the transport cell(s) from the dayside to the nightside, hence affect climate and habitability. Recent 3D model studies of Earth-

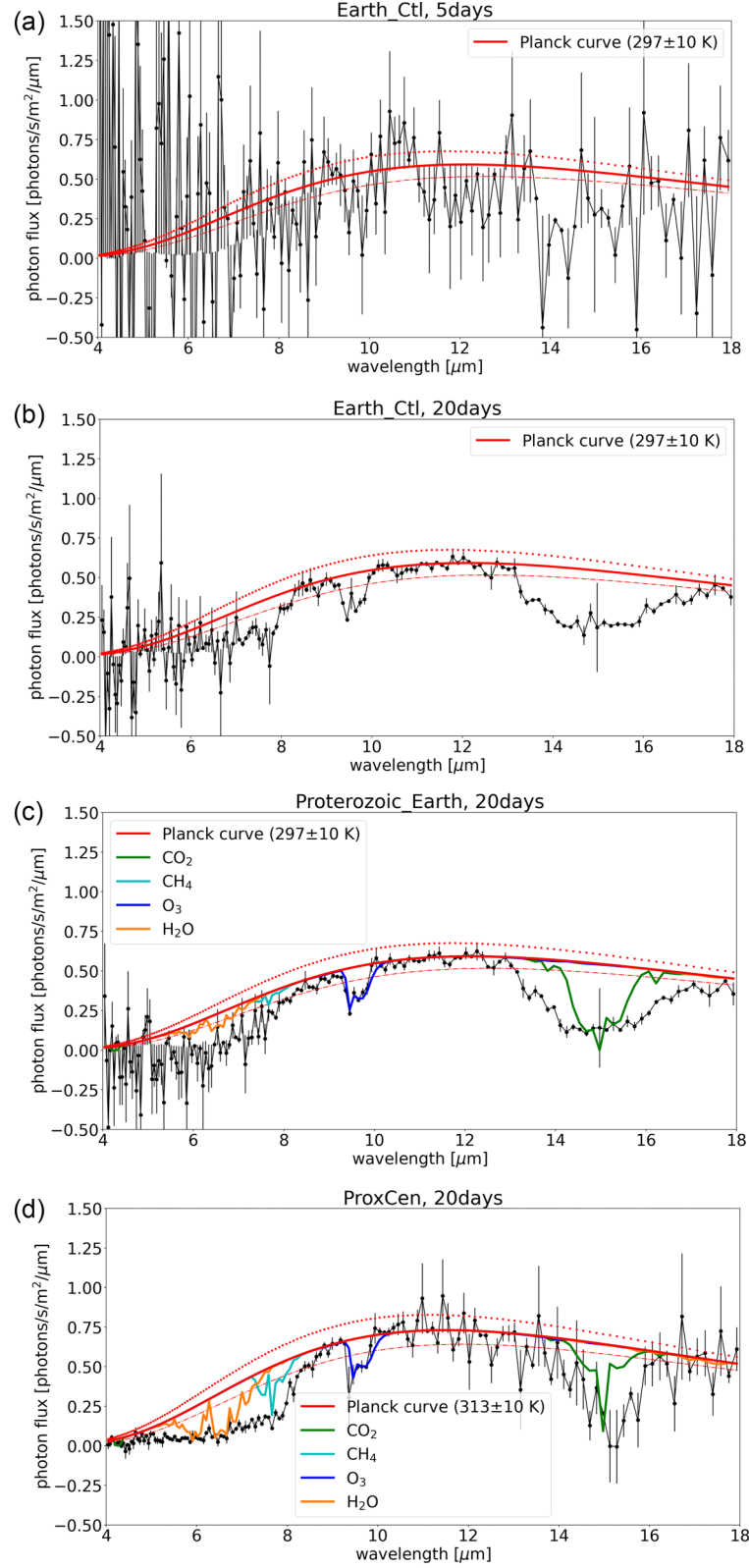


Figure 11. Emission spectra ($R = 100$) calculated with the GARLIC model (black line) fitted with Planck curves at different temperatures (red lines, see legend) for the Earth control scenario with noise for a viewing time of 5 d (panel 11a) and 20 d (panel 11b). Panel 11c is the same as 11a but for the Proterozoic Earth scenario. Panel 11d is the same as 11b but for the Proxima Centauri scenario.

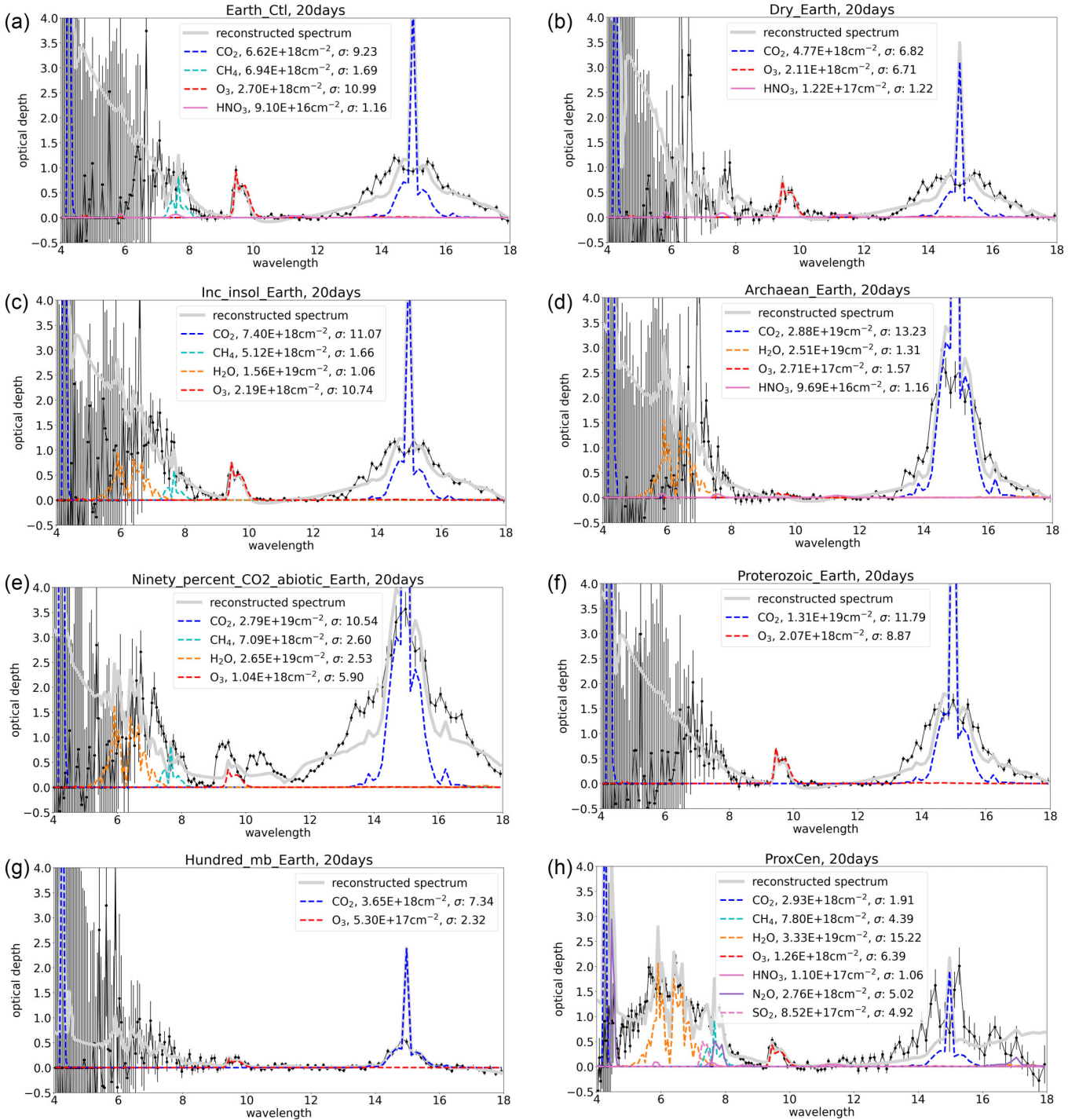


Figure 12. KIT column (averaged over the planetary disc) retrieval results for the eight scenarios, (a–h) as indicated at the top of each panel. Values shown in the legend denote one specific, randomly generated noise set-up followed by its corresponding sigma value which indicates how far the column value lies from the mean. Note that Table 3 shows the average over 100 different randomly generated noise set-ups. ‘Reconstruction’ means reconstructed spectra affected by noise based upon the retrieval. In the retrieval procedure, the square-root difference between the reconstruction and the observation is minimized (within the range of the error covariance).

like planets with coupled climate-chemistry, investigating these and related effects include M. Braam et al. (2025), H. Chen et al. (2025), and P. De Luca et al. (2024).

How could our results help guide future missions? Results suggest that planets with ages older than the Earth’s Archaean and with relatively quiet central stars could be suited for biosignature

search programs. This is because such worlds feature significant ozone layers that protect any biosphere present and means that other atmospheric biosignatures, which build up below the ozone layer in the troposphere, such as methane and nitrous oxide, would be protected from UV destruction by the overlying ozone shield. Quiet stars would also favour low atmospheric escape

Table 3. Detectability (mean) confidence level (sigma) and its standard deviation calculated by the KIT column retrieval model for 20 d viewing (see also Fig. 11). To determine the mean confidence level and its variance, 100 spectra were calculated with randomly added noise; sigma was calculated for each spectrum, and the confidence level given here is the mean of the 100 results; the error is the standard deviation of the 100 results.

Scenario	H ₂ O	HNO ₃	N ₂ O	O ₃	CO ₂	CH ₄
Earth Ctl.	0.4 ± 0.3	0.5 ± 0.4	0.5 ± 0.4	2.8 ± 0.6	2.4 ± 0.6	0.5 ± 0.4
Dry Earth	1.0 ± 0.3	0.5 ± 0.4	0.6 ± 0.4	2.0 ± 0.6	1.8 ± 0.6	0.5 ± 0.4
Inc. Insol.	0.3 ± 0.2	0.5 ± 0.4	0.6 ± 0.5	3.0 ± 0.6	2.9 ± 0.6	0.7 ± 0.7
Archaean	0.4 ± 0.2	0.4 ± 0.3	0.6 ± 0.4	0.6 ± 0.4	1.9 ± 0.5	0.6 ± 0.5
90 per cent CO ₂	0.3 ± 0.2	2.4 ± 0.5	0.7 ± 0.5	1.5 ± 0.6	1.0 ± 0.5	0.9 ± 0.6
Proterozoic	0.4 ± 0.2	0.5 ± 0.4	0.6 ± 0.4	2.4 ± 0.6	3.1 ± 0.9	0.6 ± 0.5
100mb	0.4 ± 0.3	0.5 ± 0.4	0.6 ± 0.5	0.6 ± 0.5	1.6 ± 0.6	0.6 ± 0.6
Prox-Cen	3.6 ± 0.8	0.6 ± 0.5	0.4 ± 0.3	1.0 ± 0.6	0.1 ± 0.1	1.5 ± 0.7

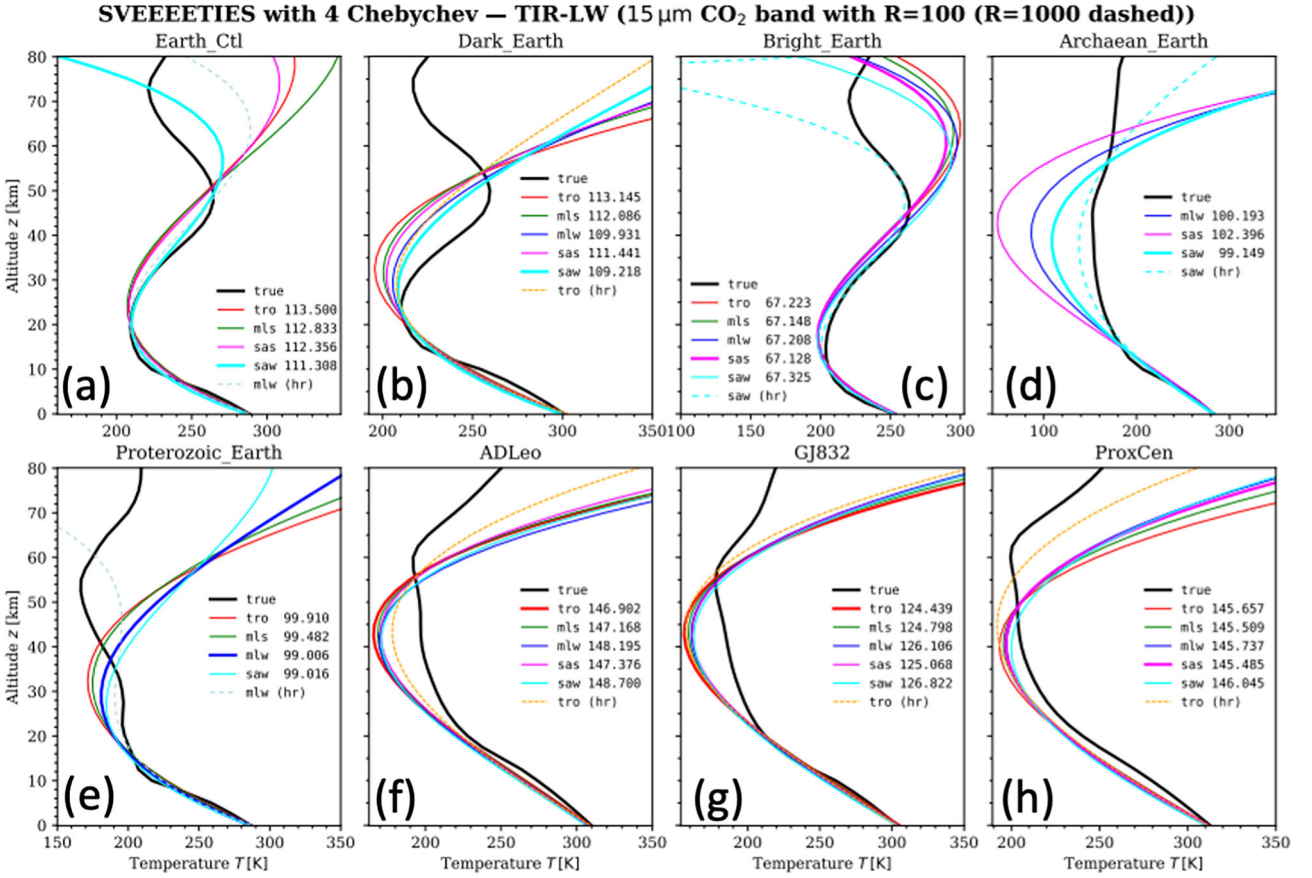


Figure 13. Atmospheric temperature profile retrievals (based on the CO₂ 15-micron band) obtained by the SVEEEETIES algorithm (see Section 2.6) for the eight scenarios shown (panels a–h) as indicated by the title of each sub-panel. In the legend, ‘true’ (solid black line) indicates the original (true) temperature profile initially used to generate the input emission spectrum. The three letter acronyms used in the legend represent the composition and initial (guess) temperature based on Earth models, where tro = tropical, mls = mid-latitude summer, mlw = mid-latitude winter, where ‘sas’ refers to sub-arctic summer and ‘saw’ refers to sub-arctic winter. The numbers show the norm of the residual spectrum (observed minus model) after convergence i.e. smaller values indicate better fits. The solid coloured lines show low resolution $R = 100$, the best fit (smallest residual norm) is indicated with double line width. The dashed lines show the best moderate resolution ($R = 1000$) fit.

rates and thicker atmospheres (>100 mb surface pressure), which feature stronger biosignature signals.

6. CONCLUSIONS

(1) Regarding biosignature profiles, ozone abundances are evident over a range of conditions. Other potential biosignatures such as CH₄, N₂O, and CH₃Cl are favoured under low UV condi-

tions e.g. planets with cooler central stars or strong atmospheric shielding.

(2) Regarding spectral signatures, CH₄ and H₂O bands are evident (i.e. discernable by inspection in the spectra) in the near-IR over a range of conditions. The O₃ fundamental band is evident for most scenarios considered but is weakened for planets with cooler central stars. The CO₂ fundamental band is evident in most scenarios considered and strengthens for low-O₂ scenarios related to upper atmosphere cooling.

(3) Regarding detectability by LIFE, CO₂ features values $> 2\sigma$ for around half the scenarios considered (Table 3) with a 20 d viewing. CH₄ detectability is challenging. O₃ is detected to $\sigma > \sim 2$ for four of the eight scenarios in Table 3, but only weakly for the Archaean and low-pressure atmosphere cases, which featured low O₃ abundances. H₂O is detected with $\sigma > \sim 3$ for only the ProxCen scenario. N₂O would not be detected. Regarding biosignature detectability for e.g. modern Earth, our results are broadly comparable with previous studies such as E. Alei et al. (2022) and D. Angerhausen et al. (2024).

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DATA AVAILABILITY

Data available on request.

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APPENDIX. RESPONSE OF SPECIES VMR TO CHANGES IN ATMOSPHERIC COLUMN (SEE DISCUSSION TO FIG. 2)

Surface emissions are emitted per unit area (cm^{-2}) per unit time (s^{-1}). Therefore, for e.g. a Super-Earth with doubled surface area compared with the Earth, the overall global surface emission (in cm^{-2}) will also be doubled. This implies a doubled emission into a doubled volume. Hence, the overall effect upon the vmr is unchanged, assuming the column extent remains unchanged. The increased gravity (at constant surface pressure) of the Super-Earth will lead to a lowering of the atmospheric column, hence a reduction in the column volume being emitted into. This results in an increase in the species vmr (e.g. CH_4) for a given surface emission. In addition, other *in situ* chemical effects could play a (smaller) role. For example, hydroxyl (OH), the main sink of CH_4 , will respond to changes in e.g. UV as the column extent changes. For three, long-lived species (N_2 , CO_2 , O_2) we fix the surface vmr (not the surface emission). This is a different precept, which assumes that the surface flux would adapt to maintain a constant vmr. Photochemical responses for these three species are however much slower ($\sim$ an order of magnitude or more) than the species (e.g. CH_4) featuring in the discussion to Figs 1 and 2.

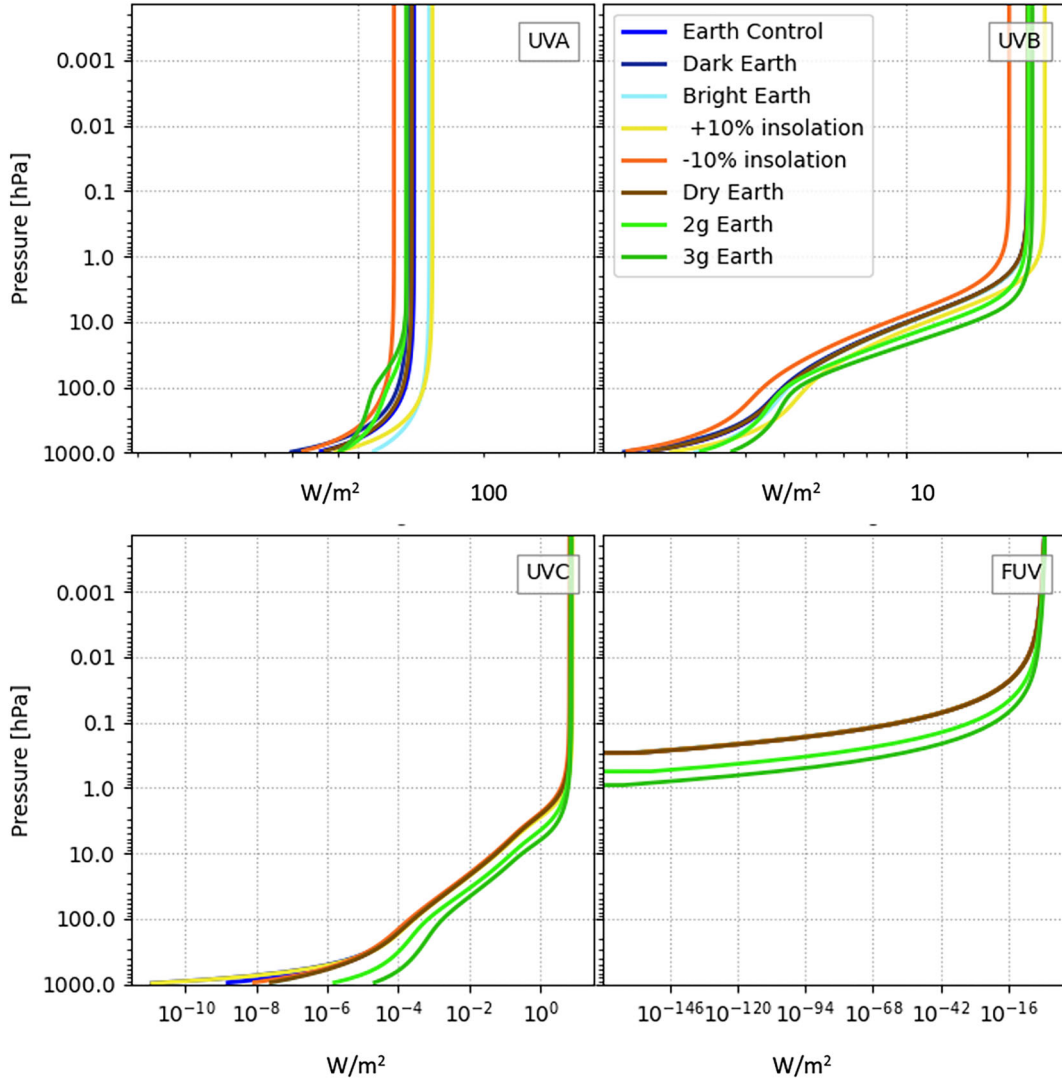


Figure A1. Modelled radiation ($W m^{-2}$) of UVA [$317.5 \text{ nm} < \lambda < 415.0 \text{ nm}$ in 1D-TERRA] (upper left), UVB [$281.7 \text{ nm} < \lambda < 317.7 \text{ nm}$] (upper right), UVC [$175.0 \text{ nm} < \lambda < 281.1 \text{ nm}$] (lower left), and FUV [$121.5 \text{ nm} < \lambda < 175.0 \text{ nm}$] (lower right).

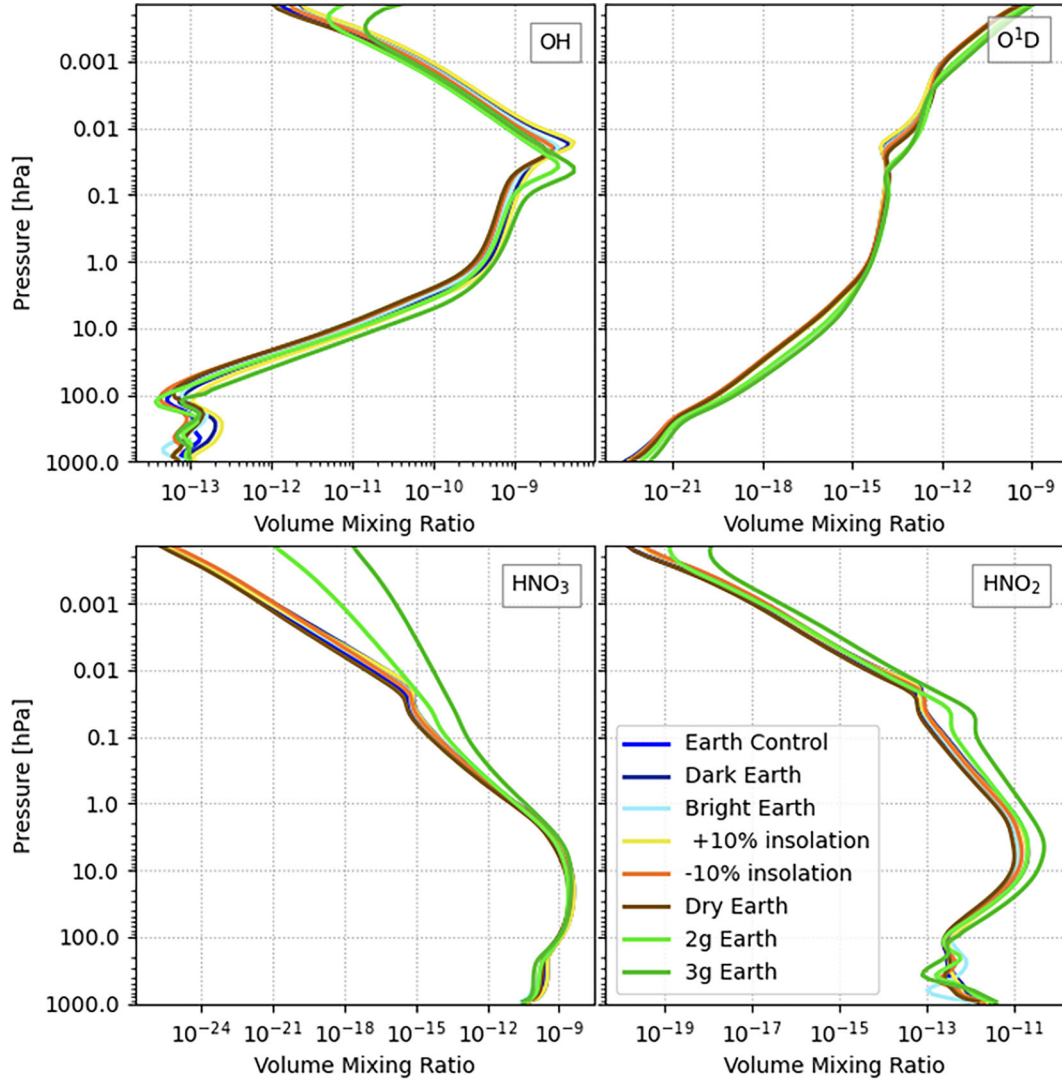


Figure A2. Hydroxyl radical (OH) (upper left), electronically excited oxygen atoms (O^1D) (upper right), nitric acid (HNO_3) (lower left), and nitrous acid (HNO_2) (lower right).

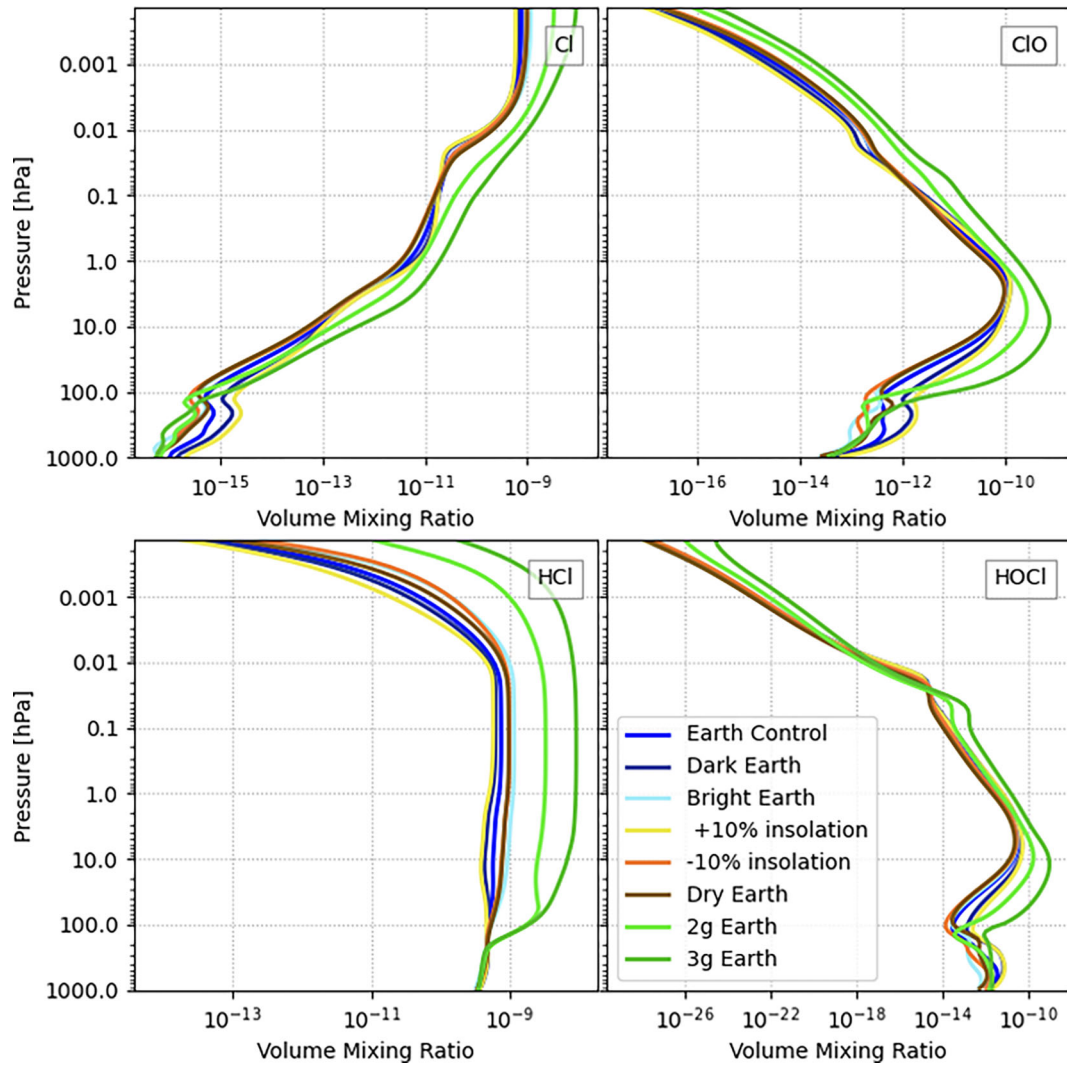


Figure A3. Atomic chlorine (Cl) (upper left), chlorine monoxide (ClO) (upper right), hydrochloric acid (HCl) (lower left), and hypochlorous acid (HOCl) (lower right).

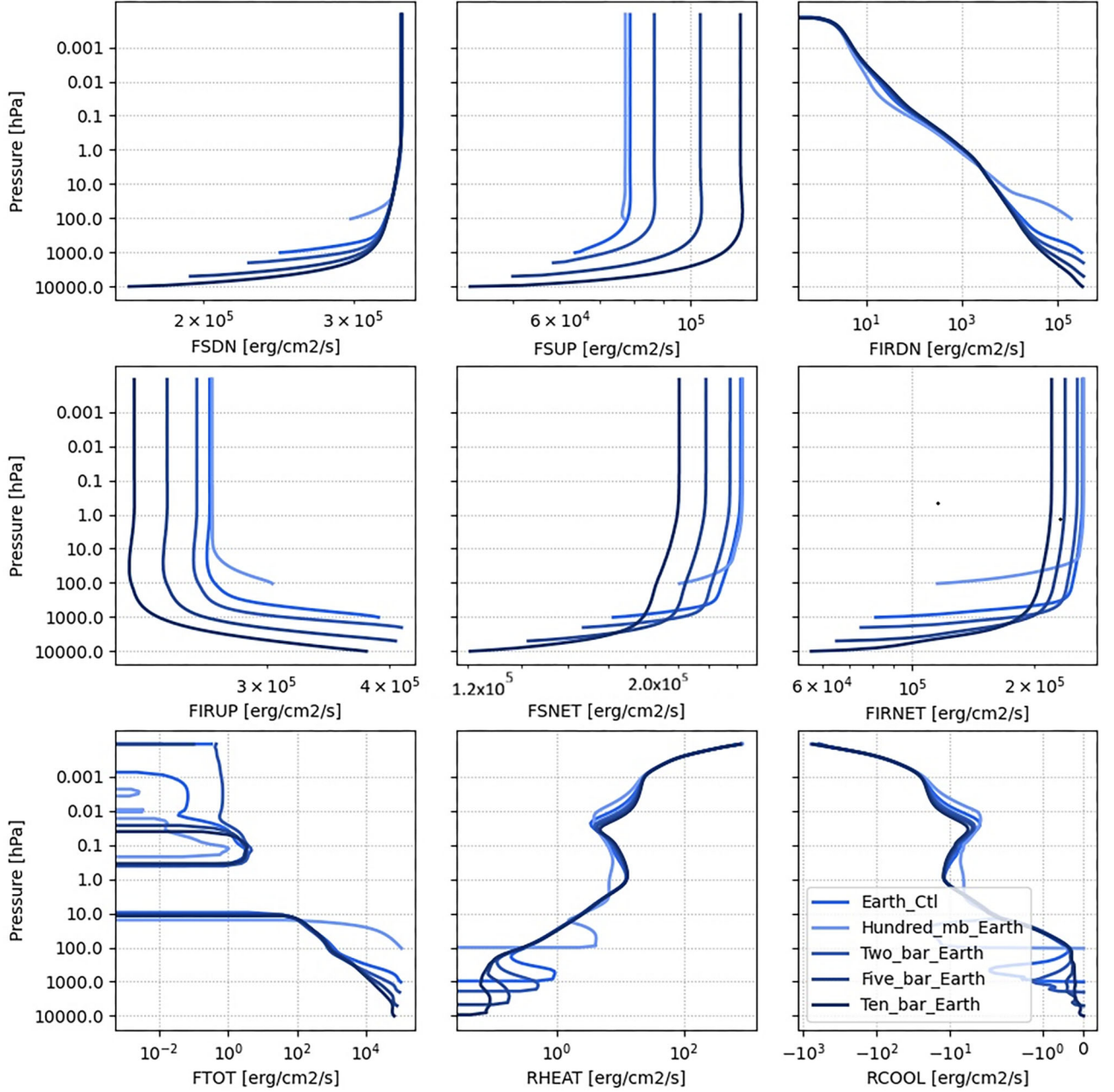


Figure A4. Panels show for the five scenarios indicated in the caption: (1) downward (incoming) shortwave (SW) fluxes (FSDN), (2) upward (outgoing) SW fluxes (FSUP), (3) downward longwave (LW) fluxes (FIRDN), (4) upward LW fluxes (FIRUP), (5) net (upwards plus downwards) SW fluxes (FSNET), (6) net (upwards plus downwards) LW fluxes (FIRNET), (7) total net fluxes (FSNET plus FIRNET), (8) total SW heating rate (RHEAT), (9) total LW cooling rate (RCOOL).

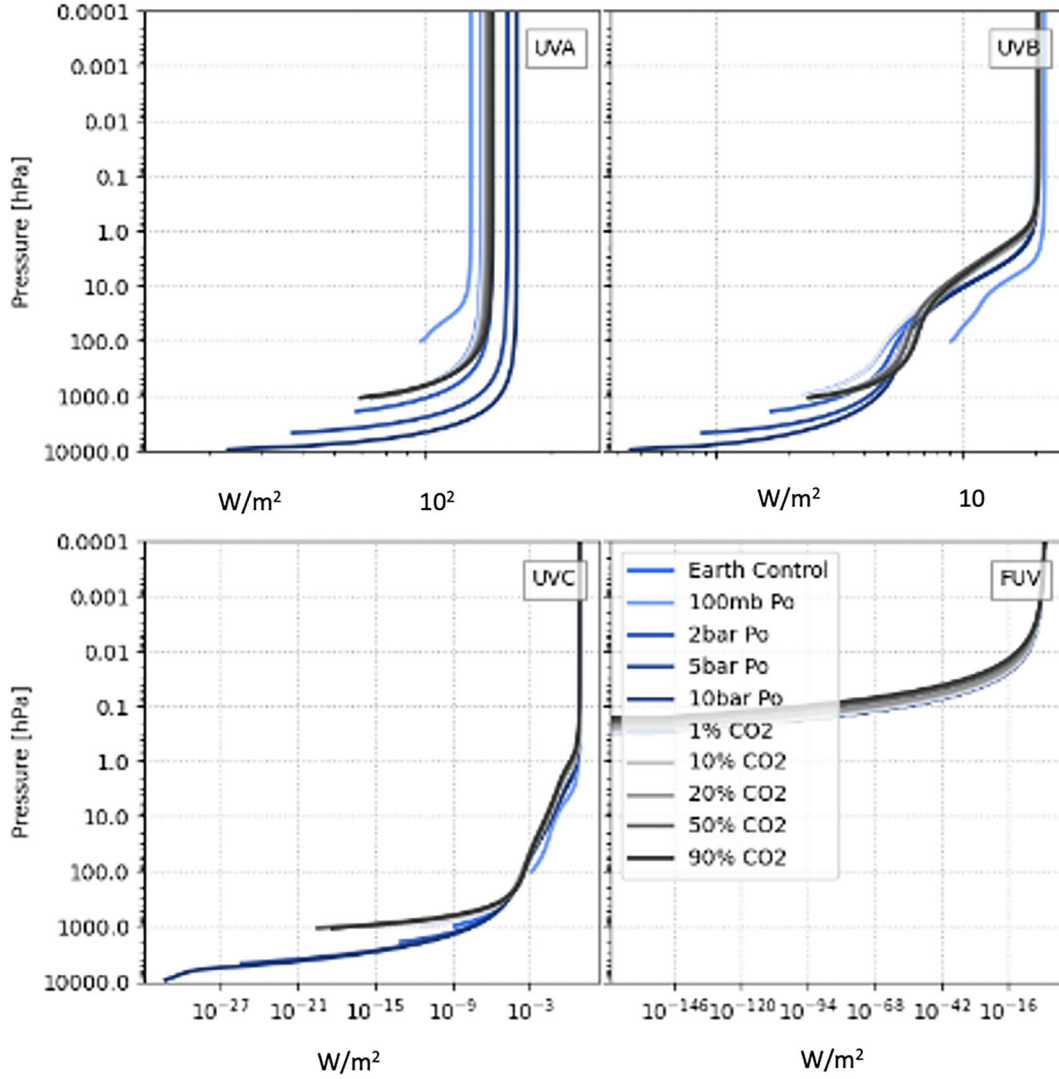


Figure A5. Modelled radiation (W m^{-2}) of UVA [$317.5 \text{ nm} < \lambda < 415.0 \text{ nm}$ in 1D-TERRA] (upper left), UVB [$281.7 \text{ nm} < \lambda < 317.7 \text{ nm}$] (upper right), UVC [$175.0 \text{ nm} < \lambda < 281.1 \text{ nm}$] (lower left), and FUV [$121.5 \text{ nm} < \lambda < 175.0 \text{ nm}$] (lower right).

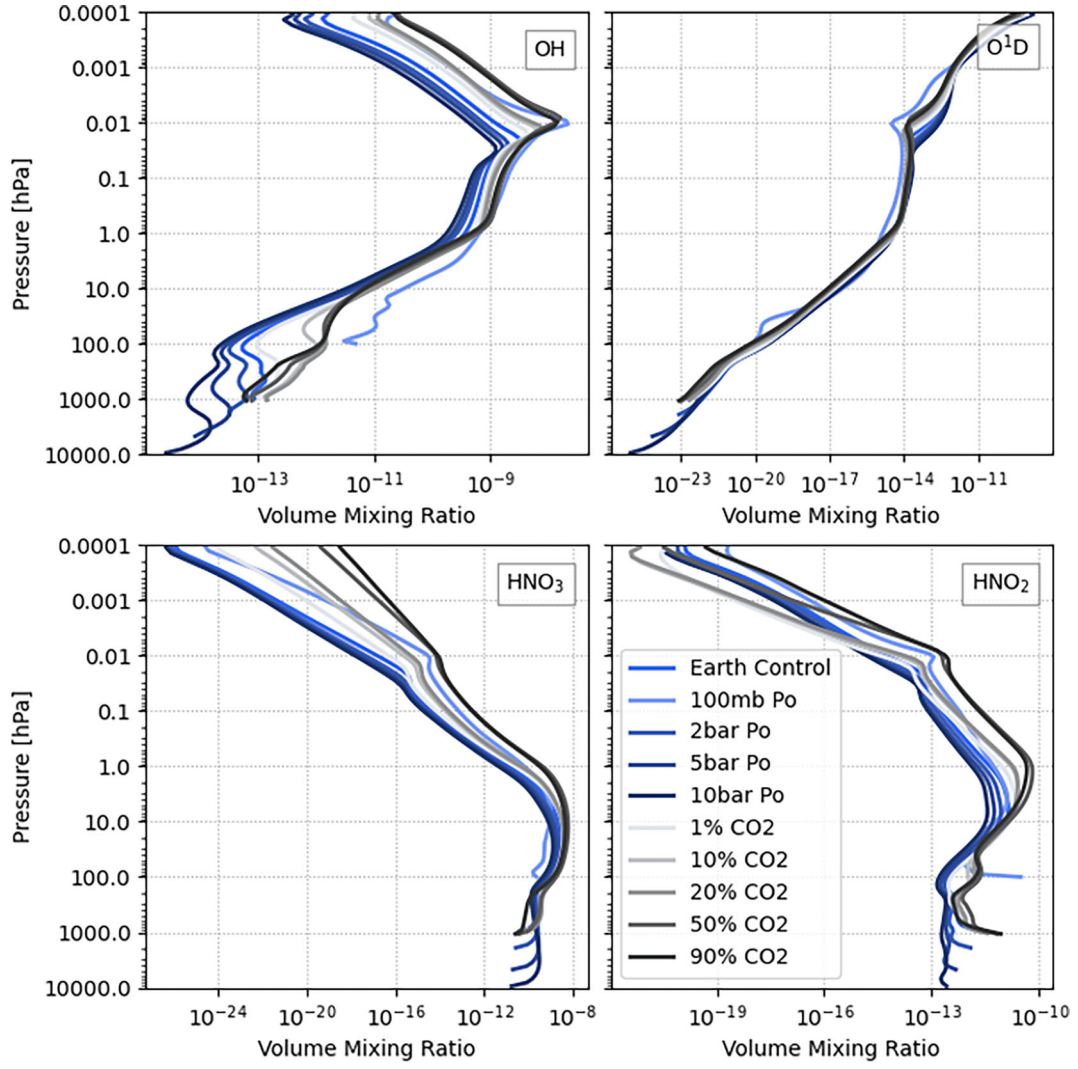


Figure A6. Hydroxyl radical (OH) (upper left), electronically excited oxygen atoms (O^1D) (upper right), nitric acid (HNO_3) (lower left), and nitrous acid (HNO_2) (lower right).

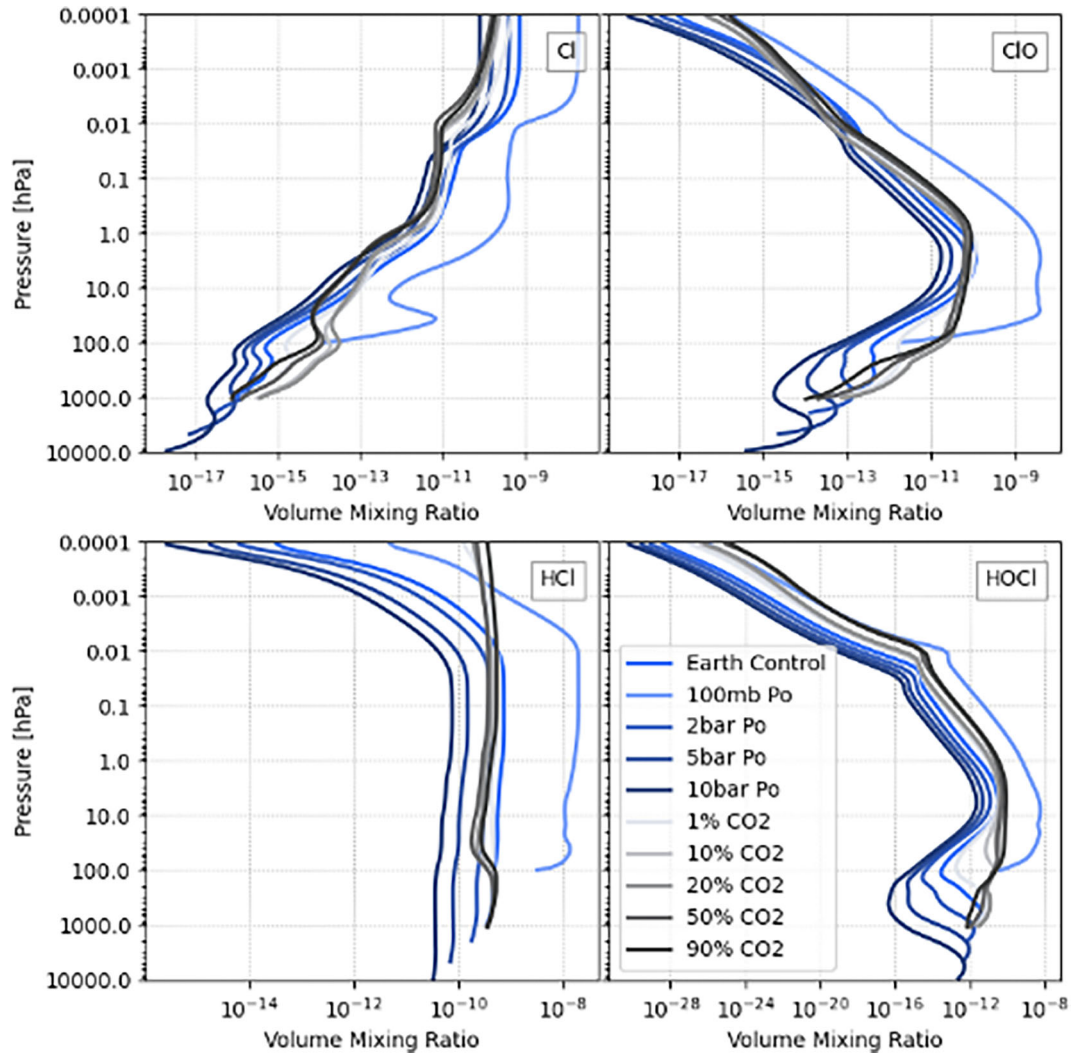


Figure A7. Atomic chlorine (Cl) (upper left), chlorine monoxide (ClO) (upper right), hydrochloric acid (HCl) (lower left), and hypochlorous acid (HOCl) (lower right).

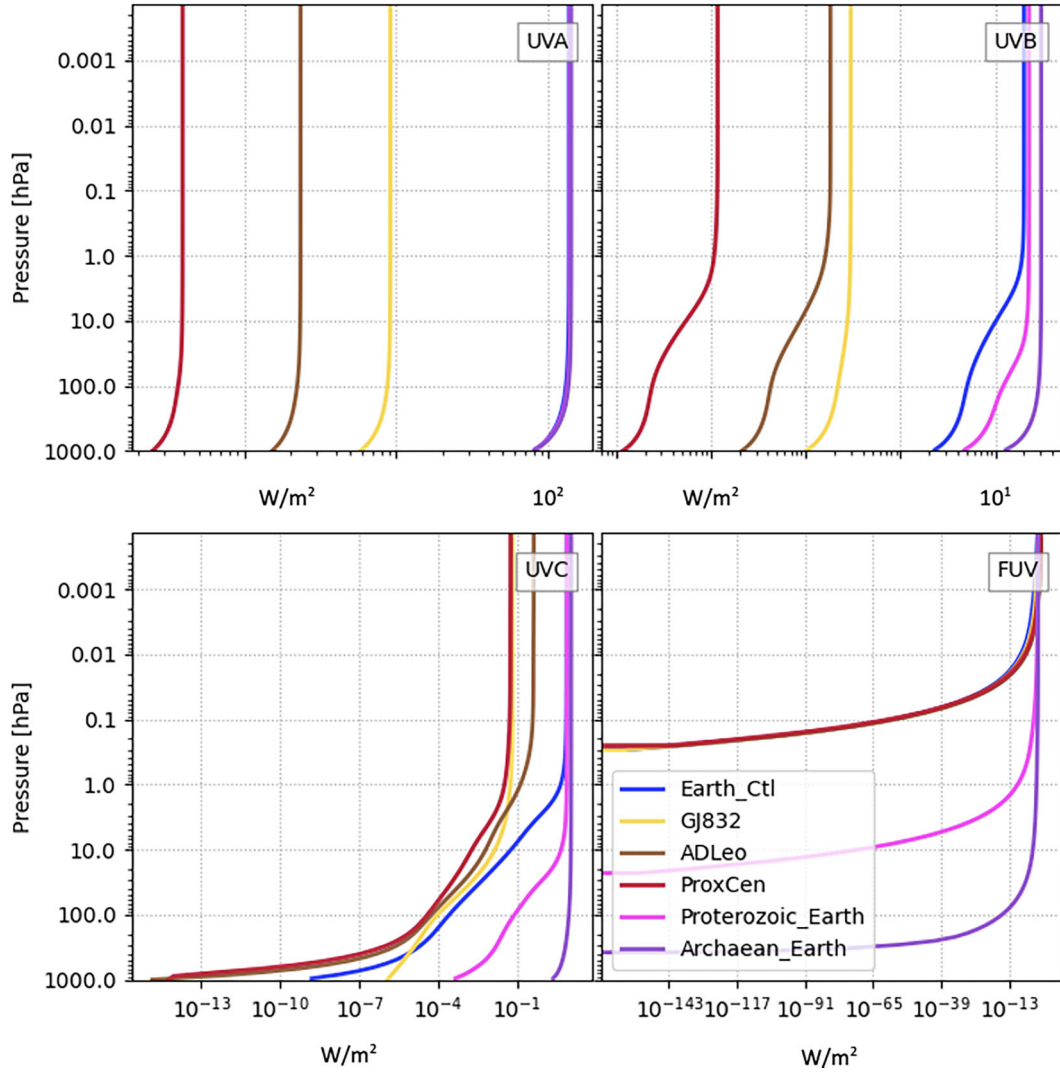


Figure A8. Modelled radiation (W m^{-2}) of UVA [$317.5 \text{ nm} < \lambda < 415.0 \text{ nm}$ in 1D-TERRA] (upper left), UVB [$281.7 < \lambda < 317.7 \text{ nm}$] (upper right), UVC [$175.0 < \lambda < 281.1 \text{ nm}$] (lower left), and FUV [$121.5 \text{ nm} < \lambda < 175.0 \text{ nm}$] (lower right) for the six scenarios indicated.

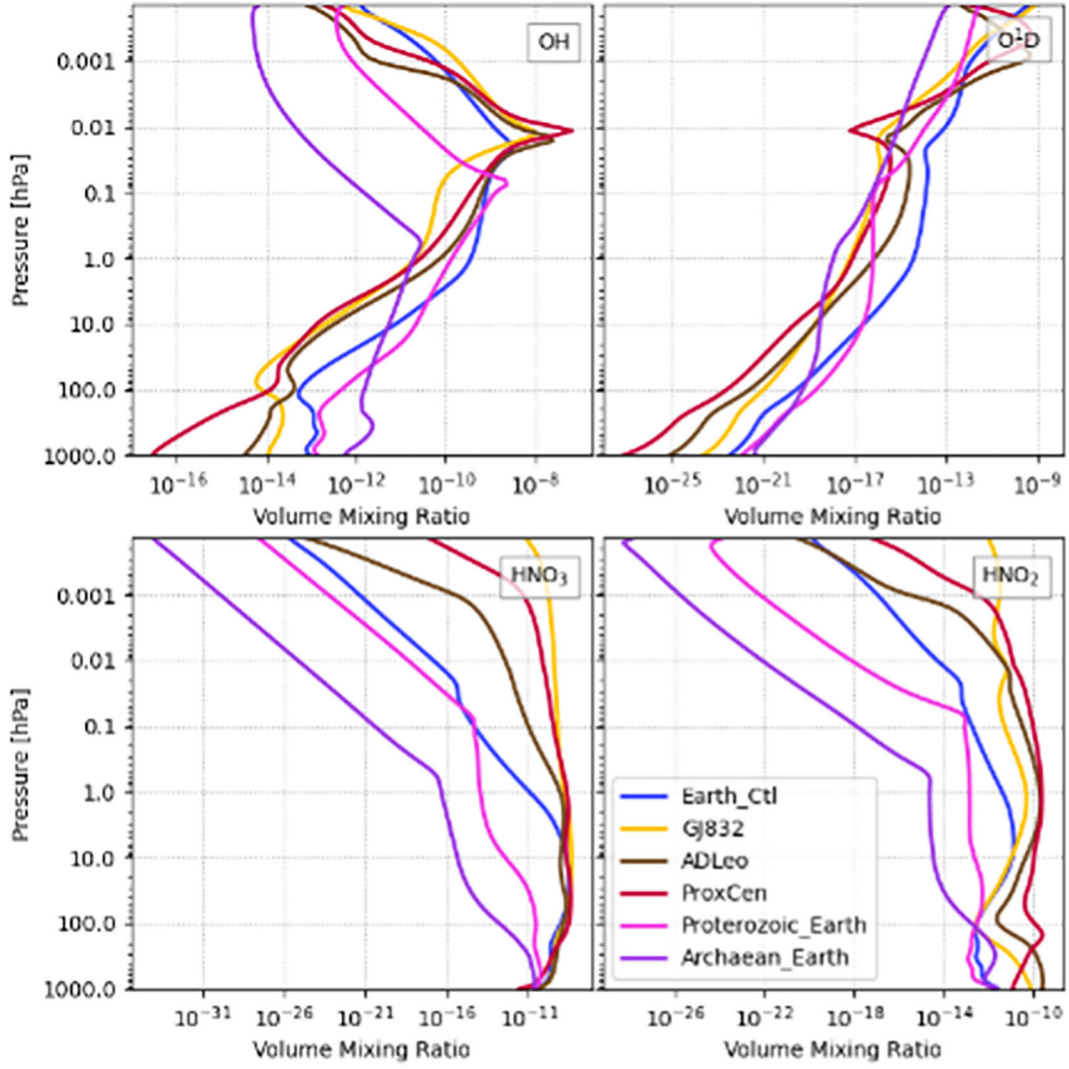


Figure A9. Hydroxyl radical (OH) (upper left), electronically excited oxygen atoms (O^1D) (upper right), nitric acid (HNO_3) (lower left), and nitrous acid (HNO_2) (lower right).

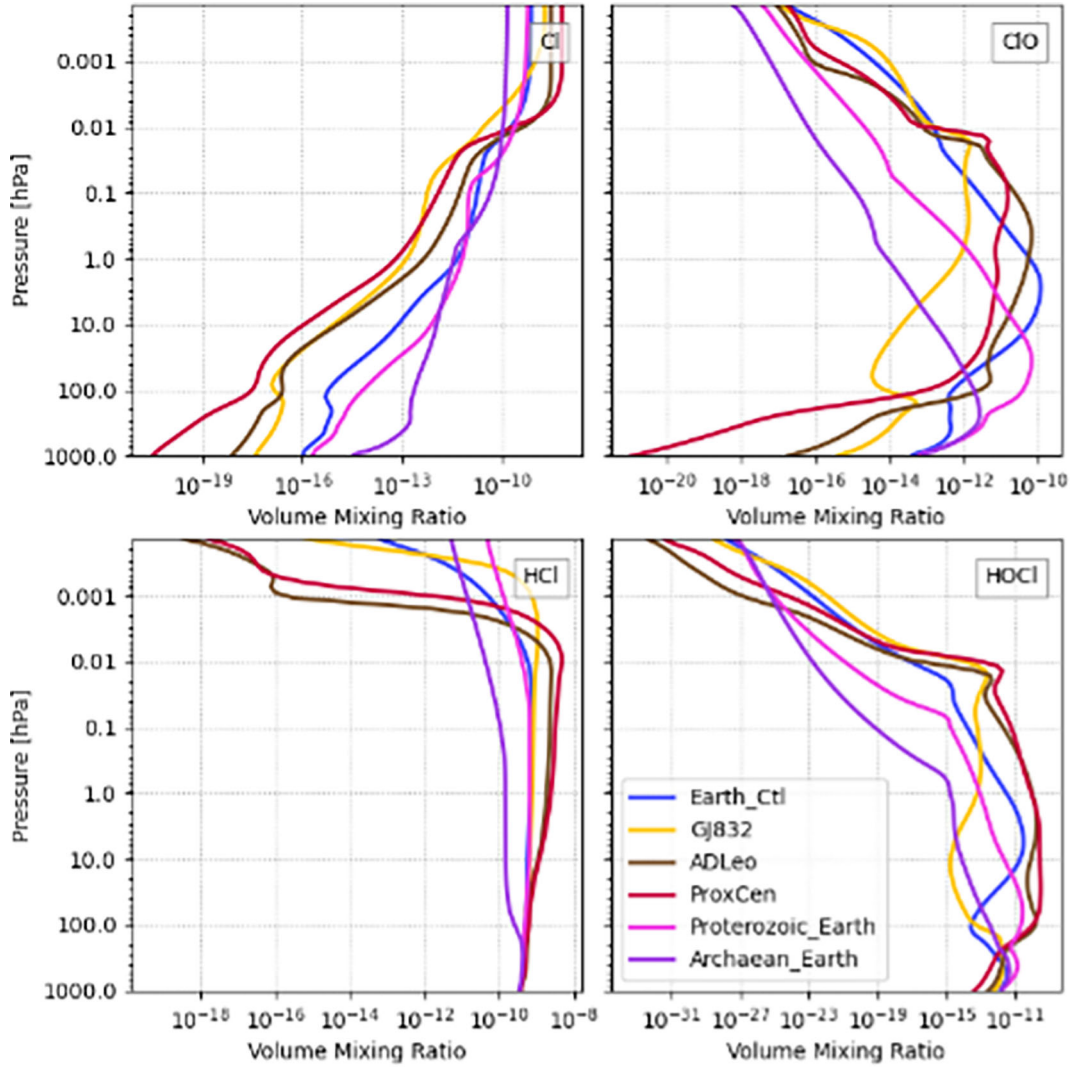


Figure A10. Atomic chlorine (Cl) (upper left), chlorine monoxide (ClO) (upper right), hydrochloric acid (HCl) (lower left), and hypochlorous acid (HOCl) (lower right).

Transmission Spectra

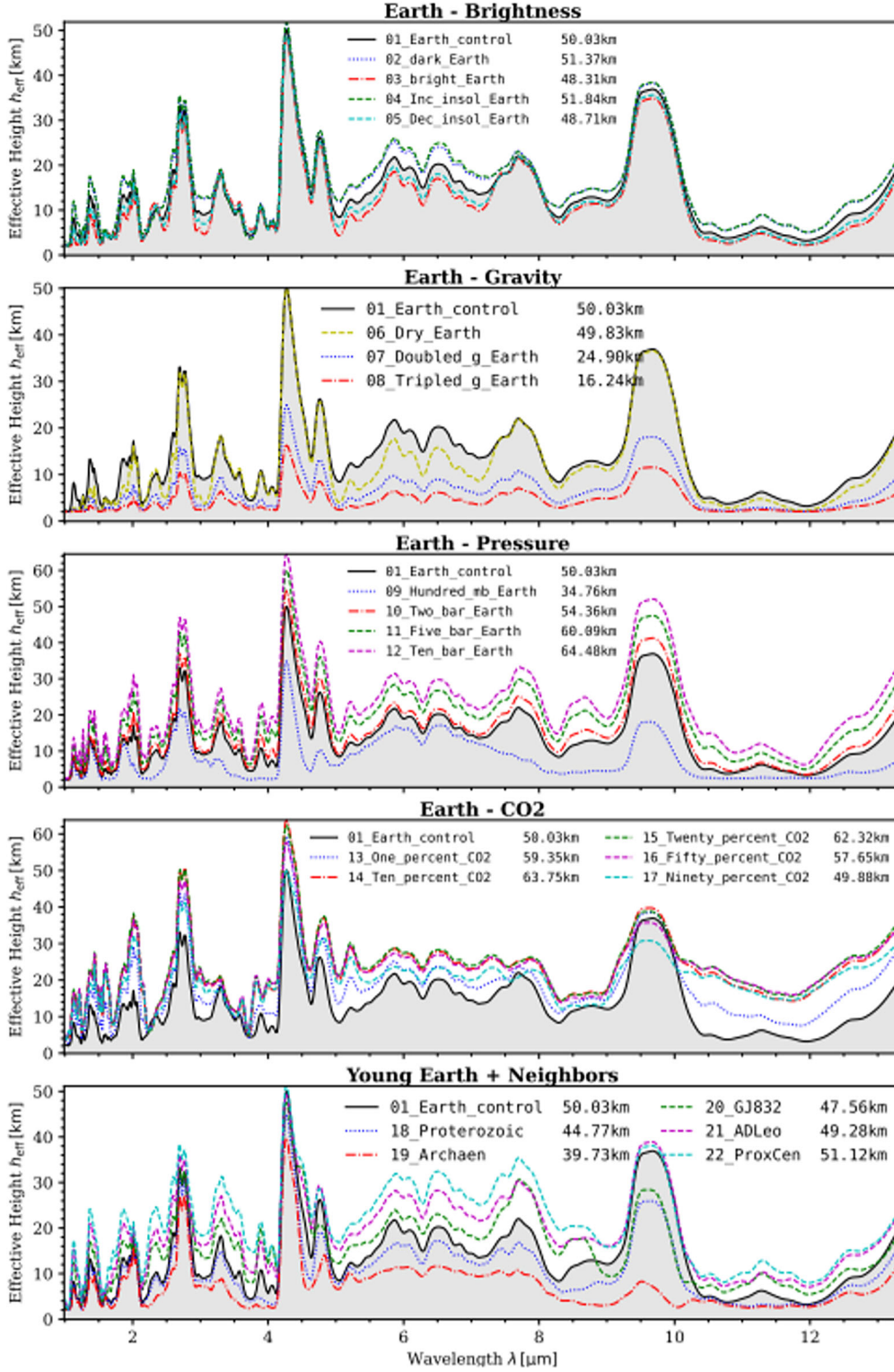


Figure A11. Spectral absorption in effective height (h_{eff} [km]) calculated by GARLIC for all scenarios from 1.0 to 13.5 microns wavelength range ($R=100$). The region below the spectral absorption for the Earth control (solid black line) is shaded grey.

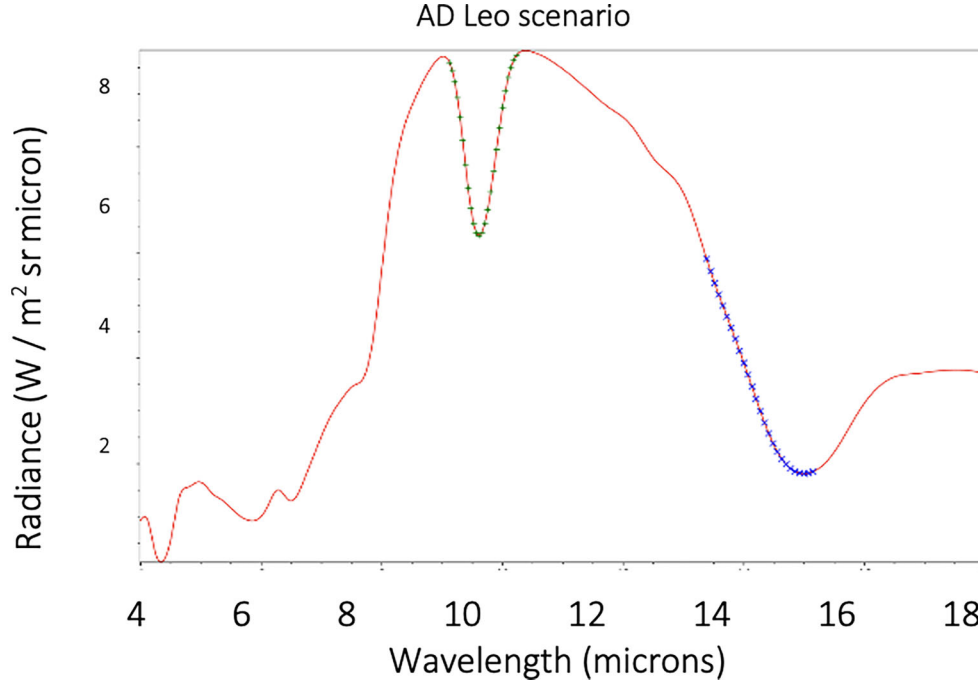


Figure A12. Illustration of the wavelength range and resolution for the fundamental O₃ band at ~ 9.6 microns (green crosses) (interval $660\text{--}750\text{ cm}^{-1}$ or $13.33\text{--}15.15$ microns) and the fundamental CO₂ band at ~ 15 microns (blue crosses) (interval $975\text{--}1100\text{ cm}^{-1}$ or $9.09\text{--}10.25$ microns) used to calculate the wavelength-integrated radiance of the band. The resulting emission was then used to calculate the differences shown in the matrix plot (Fig. 9). Data in Fig. A12 are an example case for the AD Leo scenario; note however that the wavelength range and interval of the blue and green crosses shown is the same for all scenarios.

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