Detectability of biosignatures on LHS 1140 b

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Received 12 October 2020 / Accepted 20 December 2020

ABSTRACT

Context. Terrestrial extrasolar planets around low-mass stars are prime targets when searching for atmospheric biosignatures with current and near-future telescopes. The habitable-zone super-Earth LHS 1140 b could hold a hydrogen-dominated atmosphere, and is an excellent candidate for detecting atmospheric features.

Aims. In this study we investigate how the instellation and planetary parameters influence the atmospheric climate, chemistry, and spectral appearance of LHS 1140 b. We study the detectability of selected molecules, in particular potential biosignatures, with the upcoming James Webb Space Telescope (JWST) and Extremely Large Telescope (ELT).

Methods. In the first step we used the coupled climate–chemistry model 1D-TERRA to simulate a range of assumed atmospheric chemical compositions dominated by molecular hydrogen (H₂) and carbon dioxide (CO₂). In addition, we varied the concentrations of methane (CH₄) by several orders of magnitude. In the second step we calculated transmission spectra of the simulated atmospheres and compared them to recent transit observations. Finally, we determined the observation time required to detect spectral bands with low-resolution spectroscopy using JWST, and the cross-correlation technique using ELT.

Results. In H₂-dominated and CH₄-rich atmospheres oxygen (O₂) has strong chemical sinks, leading to low concentrations of O₂ and ozone (O₃). The potential biosignatures ammonia (NH₃), phosphine (PH₃), chloromethane (CH₂Cl), and nitrous oxide (N₂O) are less sensitive to the concentration of H₂, CO₂, and CH₄ in the atmosphere. In the simulated H₂-dominated atmosphere the detection of these gases might be feasible within 20 to 100 observation hours with ELT or JWST when assuming weak extinction by hazes.

Conclusions. If further observations of LHS 1140 b suggest a thin, clear, hydrogen-dominated atmosphere, the planet would be one of the best known targets to detect biosignature gases in the atmosphere of a habitable-zone rocky exoplanet with upcoming telescopes.

Key words. planets and satellites: terrestrial planets – planets and satellites: detection – planets and satellites: composition – planets and satellites: atmospheres – techniques: spectroscopic – astrochemistry

1. Introduction

The nearby temperate super-Earth LHS 1140 b (Dittmann et al. 2017; Ment et al. 2019) is an exciting target for atmospheric characterization. Morley et al. (2017) assumed Venus-, Titan-, and Earth-like atmospheres for LHS 1140 b. Their results suggest that atmospheric characterization with the James Webb Space Telescope (JWST) could be possible, although challenging.

A recent study of the temporal radiation environment of the LHS 1140 system suggests that the planet receives relatively constant near-ultraviolet (NUV; 177–283 nm) flux <2% compared to that of Earth (Spinelli et al. 2019). The results of Chen et al. (2019) suggest that LHS 1140 b might be stable against complete ocean desiccation due to the low UV activity of the host star, which would bode well for its habitability. However, Chen et al. (2019) assumed a rather low UV flux for the star, which might lead to an underestimation of the water loss. Furthermore, due to the extended pre-main-sequence phase of M dwarfs (see, e.g., Baraffe et al. 2015; Luger & Barnes 2015), LHS 1140 b may have experienced extreme water loss before the star entered the main-sequence phase (see, e.g., Luger & Barnes 2015).

Assuming an Earth-like atmosphere with updated sea-ice parameterization, the 3D model study of Yang et al. (2020) suggests a reduced surface ocean on LHS 1140 b (from 12 to 3% surface coverage). Diamond-Lowe et al. (2020) observed two transits of LHS 1140 b with the twin Magellan Telescopes, but their analysis suggests that a precision increased by a factor of about 4 was needed for the detection of a cloudless hydrogen atmosphere, for example, present at amounts consistent with the bulk density. Recently, Edwards et al. (2021) presented spectrally resolved observations of LHS 1140 b using the G141 grism of the Wide Field Camera 3 (WFC3) on the Hubble Space Telescope (HST). Their results suggest that the planet may host a clear H₂-dominated atmosphere and may show evidence of an absorption feature at 1.4 μm.

The processes affecting the climates and compositions of super-Earths such as LHS 1140 b are not well known. Evidence has been found that there is a dip in the radius distribution of extrasolar planets at 1.5–2.0 R⊕ (see, e.g., Owen & Wu 2013; Fulton et al. 2017; Van Eylen et al. 2018; Hardegree-Ullman et al. 2020). With a radius of ~1.7 R⊕, LHS 1140 b lies within this “radius valley” (Ment et al. 2019), which is interpreted as the transition between predominantly rocky planets and volatile-rich planets. A number of studies have investigated the origin of the radius valley (see, e.g., Owen & Wu 2013, 2017; Lee et al. 2014;
Lopez & Rice 2018; Ginzburg et al. 2018; Gupta & Schluchter 2019). LHS 1140 b is not expected to have a large H₂–He envelope due to its high bulk density of \( \rho \), of 7.5 ± 1.0 cm\(^{-3} \) (Ment et al. 2019). However, massive super-Earths might retain small residual H\(_2\) atmospheres at the end of the core-powered mass loss (see, e.g., Ginzburg et al. 2016; Gupta & Schluchter 2019).

In H\(_2\)-dominated atmospheres significant heating could be induced by self- and foreign H\(_2\) collision induced absorption (CIA; e.g., Pierrehumbert & Gaidais 2011; Ramirez & Kaltenegger 2017). Regarding the composition, lessons from the solar system gas giants (Yung & DeMore 1999, and references therein) suggest ammonia (NH\(_3\)) and phosphine (PH\(_3\)) chemistry, as well as pathways starting with methane (CH\(_4\)) forming long-chain hydrocarbons that can condense to form hazes, and pathways destroying long-chain hydrocarbons driven mainly by initial reaction with atomic hydrogen (H) from extreme UV (EUV) photolysis of H\(_2\). In exoplanetary science Hu & Seager (2014), among others, studied the photochemical responses of hydrogen atmospheres on super-Earths; Line et al. (2011) discussed processes controlling the partitioning between CH\(_4\) and CO on GJ 436 b; and recently Lavvas et al. (2019) studied the effects of photochemistry, mixing, and hazes on GJ 1214 b.

Clouds and hazes can obscure the observed spectrum of the planetary atmosphere below the top of the haze or cloud layer. Arney et al. (2016, 2017) used a 1D climate–chemistry model to simulate the photochemically driven formation of organic hazes in the atmosphere of early Earth and exoplanets located in the habitable zones (HZs) of their host stars. They concluded that the concentration of C\(_2\)H\(_4\) has a large impact on haze formation, and propose that a hydrocarbon haze may be a biosignature on planets with substantial levels of CO\(_2\).

The detection of potential biosignature gases like oxygen (O\(_2\)), nitrous oxide (N\(_2\)O), or chloromethane (CH\(_3\)Cl) in an Earth-like or CO\(_2\)-dominated atmosphere will be challenging using transmission or emission spectroscopy (see, e.g., Schwieterman et al. 2018; Batalha et al. 2018; Wunderlich et al. 2019; Lustig-Yaeger et al. 2019). The characterization of an H\(_2\) atmosphere is more favorable due to the lower mean molecular weight leading to larger spectral features. In such an atmosphere several potential biosignatures might be detectable including NH\(_3\), dimethyl sulfide (DMS), CH\(_3\)Cl, PH\(_3\), and N\(_2\)O (Seager et al. 2013a;b; Schwieterman et al. 2018; Sousa-Silva et al. 2020).

In this work we apply the steady-state, cloud-free, radiative-convection photochemistry model 1D-TERRA (Scheuer et al. 2020; Wunderlich et al. 2020) together with the theoretical spectral model GARLIC (Schreier et al. 2014) to simulate a range of CO\(_2\), H\(_2\)-He atmospheres (and mixtures thereof), as well as atmospheric spectra for LHS 1140 b. The central aim of our work is to investigate potential atmospheres of this super-Earth and determine the detectability of key atmospheric features, in particular potential biosignatures, in the context of the forthcoming JWST and Extremely Large Telescope (ELT).

Section 2 introduces the climate–photochemistry model 1D-TERRA, the line-by-line spectral model GARLIC, and the signal-to-noise ratio (S/N) models for JWST and ELT. In Sect. 3 we first show the results of the atmospheric modeling and the resulting transmission spectra, followed by the results of the S/N calculations. We summarize and conclude our results in Sect. 4.

2. Methodology

2.1. System parameter and stellar input spectrum

LHS 1140 is a close-by M4.5-type main-sequence red dwarf 14.993 ± 0.015 pc away from the Earth (Gaia Collaboration 2018) with an effective temperature \( (T_{\text{eff}}) \) of 3219 ± 39 K, a radius \( (R) \) of 0.2139 ± 0.0041 \( R_\odot \), and a mass \( (M) \) of 0.179 ± 0.014 \( M_\odot \) (Ment et al. 2019). The star is known to host two rocky planets, LHS 1140 b and LHS 1140 c (Dittmann et al. 2017; Ment et al. 2019). In this study we simulate the potential atmosphere of the habitable zone planet LHS 1140 b by using a radius of 1.727 ± 0.032 \( R_\oplus \), a mass of 6.98 ± 0.89 \( M_\oplus \), and a surface gravity \( (g) \) of 23.7 ± 2.7 m s\(^{-2} \) (Ment et al. 2019). We do not expect that our results would change significantly when using the slightly lower planetary mass of 6.48 ± 0.46 \( M_\oplus \) suggested by Lillo-Box et al. (2020). The planet receives an incident flux of 0.503 ± 0.03 \( S_\odot \) and orbits its host star in ∼24.7 days.

The stellar spectrum has not been measured for LHS 1140. However, the FUV\(1344-1766\AA\)/NUV\(711-2831\AA\) ratio was determined to be 0.303 ± 0.080 (Spinelli et al. 2019). In the UV range up to 400 nm, we use the adapted panchromatic spectral energy distribution (SED) of Proxima Centauri from the MUSCLES database version 22 (France et al. 2016; Loyd et al. 2016) with a value of 0.313. In the visible and near-infrared (NIR) we take the SED from GJ 1214 with stellar parameters similar to LHS 1140 \( (T_{\text{eff}} = 3252 ± 20 \, K, R = 0.211 \pm 0.011 \, R_\oplus, M = 0.176 \pm 0.009 \, M_\oplus, \) Anglada-Escudé et al. 2013).

2.2. Model description and updates

In this study we use the radiative-convective photochemistry model 1D-TERRA. The code dates back to early work by Kasting & Ackerman (1986), Pavlov et al. (2000), and Segura et al. (2003) and has been considerably extended by Grenfell et al. (2007, 2013), Rauer et al. (2011), von Paris et al. (2011, 2015), and Gebauer et al. (2017), among others. Recently, a major update of the climate radiative transfer module (called REDFOX; Scheuer et al. 2020) and chemistry module (called BLACKWOLF; Wunderlich et al. 2020) enabled CO\(_2\)- and H\(_2\)-dominated atmospheres to be consistently simulated.

REDFOX includes absorption values of 20 molecules\(^1\) using spectroscopic cross sections from the HITRAN 2016 line list (Gordon et al. 2017) and 81 molecules using UV and VIS cross sections mainly taken from the MPI Mainz Spectral Atlas (Keller-Rudek et al. 2013) as described in Scheuer et al. (2020) and Wunderlich et al. (2020). Additionally, Rayleigh scattering of eight molecules\(^2\) and Mlawer-Tobin-Clough-Kneizys-Davies absorption (MT_CKD; Mlawer et al. 2012) and CIs of H\(_2\)-H\(_2\), H\(_2\)-He, CO\(_2\)-H\(_2\), CO\(_2\)-CH\(_4\), and CO\(_2\)-CO\(_2\) are considered (see Scheuer et al. 2020, for details).

The globally averaged zenith angle is set to 60° in the climate module and 54.5° in the chemistry module in order to fit the observed O\(_3\) column of ∼30 Dobson Units (DU) on Earth (see, e.g., de Grandpré et al. 2000; Thouret et al. 2006). The atmosphere in the climate module is divided into 101 pressure levels and the chemistry module into 100 pressure layers. The eddy diffusion profile can be calculated according to the parameterization shown in Wunderlich et al. (2020), or set to a given profile. Unless indicated otherwise, we use a parameterized eddy diffusion profile. The photochemical module accounts for dry and wet deposition, as well as surface emission fluxes and atmospheric escape (see details in Wunderlich et al. 2020). For wet deposition we use the parameterization of Giorgi & Chameides (1985) and the tropospheric lightning emissions of nitrogen oxides, NO\(_x\).

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1. CH\(_3\)Cl, CH\(_4\), CO, CO\(_2\), H\(_2\), HCl, HCN, HNO\(_3\), HO\(_2\), HOCI, N\(_2\), N\(_2\)O, NH\(_3\), NO, NO\(_2\), O\(_3\), OH, and SO\(_2\).

2. CO, CO\(_2\), H\(_2\)O, N\(_2\), O\(_3\), H\(_2\)He, and CH\(_4\).
(here defined as NO + NO₂), which are based on the Earth lightning model of Chameides et al. (1977).

In the current paper we additionally introduced some minor updates compared to the photochemical model described in Wunderlich et al. (2020). Recently, the water (H₂O) cross section between 186–230 nm has been measured by Ranjan et al. (2020) for a temperature of 292 K. We use this new cross section data in the current study. However, the weak NUV flux of M dwarfs suggests that the water photolysis is not affected significantly by the use of the new measurements (see, e.g., Wunderlich et al. 2019).

Recently, Greaves et al. (2020a) found evidence of phosphine (PH₃) absorption in the atmosphere of Venus. The presence of detectable amounts of PH₃ is still debated in the literature (Snellen et al. 2020; Thompson 2021; Encrenaz et al. 2020; Villanueva et al. 2020; Mogul et al. 2020; Greaves et al. 2020b,c), and the chemical and biological processes leading to its production are not well known (Greaves et al. 2020a; Bains et al. 2020; Lingam & Loeb 2020). However, Sousa-Silva et al. (2020) suggest that in H₂- and CO₂-dominated atmospheres chemical sinks of PH₃ are reduced compared to Earth, favoring a potential detection in such an environment. In the atmosphere of gas giants, where the pressure and temperature and the concentration of H₂ are sufficiently high, the thermodynamical formation of PH₃ is favored (see, e.g., Visscher et al. 2006). For rocky, potentially habitable planets these conditions are not expected making PH₃ a reasonable candidate biosignature gas in a reduced atmosphere.

The chemical network of BLACKWOLF, as presented in Wunderlich et al. (2020), did not include the chemical production and destruction of PH₃. Hence, we consider in the present work 16 additional phosphorous containing reactions (see Table 1). To calculate the wet deposition of PH₃ we use the Henry’s law constant from Fu et al. (2013). We do not consider a sink reaction for tetraphosphorus (P₄). At low temperatures P₄ is expected to sublimate without undergoing chemical reaction or photolysis (see, e.g., Kaye & Strobel 1984). Hence, we assume that all P₄ is deposited or removed from the atmosphere in order to avoid a runaway effect.

With the new chemical reactions from Table 1 we repeated the validation of modern Earth with 1D-TERRA shown in Wunderlich et al. (2020). The additional consideration of PH₃ has no significant impact on the concentration of key species in the atmosphere of modern Earth. PH₃ was measured locally on Earth with concentrations ranging between 1 × 10⁻¹⁵ (ppq) and 1 × 10⁻¹⁹ (ppb) (see Pasek et al. 2014; Bains et al. 2019; Sousa-Silva et al. 2020, and references therein). 1D-TERRA suggests a global and annual mean surface mixing ratio of 1 × 10⁻¹² (1 ppt) when using an assumed surface emission flux of 1 × 10⁸ molecules cm⁻² s⁻¹.

In addition to the validation of 1D-TERRA against modern Earth, in Scheucher et al. (2020) and Wunderlich et al. (2020) the climate and chemistry modules were validated against Mars- and Venus-like conditions to show that the model is able to predict consistently N₂-O₂ and CO₂-dominated atmospheres. In this work we validate the model against H₂-dominated and CH₄-rich atmospheres; the simulation of the atmosphere of Neptune can be found in Appendix A and that of Titan in Appendix B.

### Table 1. Phosphorous containing reactions added to the photochemical reaction scheme.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Reaction coefficients</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>PH₃+O¹D → PH₂+OH</td>
<td>4.75 × 10⁻¹¹</td>
<td>(1)</td>
</tr>
<tr>
<td>PH₃+OH → PH₂+H₂O</td>
<td>2.71 × 10⁻¹¹, 1e⁻¹⁵⁵/T</td>
<td>(2)</td>
</tr>
<tr>
<td>PH₃+O → PH₂+OH</td>
<td>9.95 × 10⁻³⁸</td>
<td>(3)</td>
</tr>
<tr>
<td>PH₃+H → PH₂+H₂</td>
<td>7.22 × 10⁻¹¹, 1e⁻⁸⁸⁶/T</td>
<td>(4)</td>
</tr>
<tr>
<td>PH₃+Cl → PH₁+HCl</td>
<td>2.36 × 10⁻¹⁰</td>
<td>(5)</td>
</tr>
<tr>
<td>PH₃+N → PH₂+NH</td>
<td>4.00 × 10⁻¹⁴</td>
<td>(6)</td>
</tr>
<tr>
<td>PH₃+N₂H → PH₂+NH₃</td>
<td>1.00 × 10⁻¹₂, 1e⁻⁹²⁸/T</td>
<td>(7)</td>
</tr>
<tr>
<td>PH₃+H₂ → PH₂+NH₃</td>
<td>6.20 × 10⁻¹¹, 1e⁻³¹⁸/T</td>
<td>(8)</td>
</tr>
<tr>
<td>PH₃+H → PH₂+H₂</td>
<td>1.50 × 10⁻¹⁰, 1e⁻⁴₁⁶/T</td>
<td>(8)</td>
</tr>
<tr>
<td>P₄+H → P₃+H₄</td>
<td>5.00 × 10⁻¹¹, 1e⁻⁴⁰⁰/T</td>
<td>(8)</td>
</tr>
<tr>
<td>PH₂+H₄+M → PH₃+M</td>
<td>3.70 × 10⁻¹⁰, 1e⁻³⁴⁰/T</td>
<td>(8)</td>
</tr>
<tr>
<td>PH₃+H₄+M → PH₄+M</td>
<td>3.00 × 10⁻³⁶, N</td>
<td>(8)</td>
</tr>
<tr>
<td>P₄+P₄+M → P₃+M</td>
<td>1.40 × 10⁻³³, 1e⁻⁴⁰⁰/T · N</td>
<td>(8)</td>
</tr>
<tr>
<td>P₄+H+M → PH₄+M</td>
<td>3.40 × 10⁻³³, 1e⁻³⁷⁷/T · N</td>
<td>(8)</td>
</tr>
<tr>
<td>P₄+P₄+M → P₃+M</td>
<td>1.40 × 10⁻³³, 1e⁻⁴⁰⁰/T · N</td>
<td>(9)</td>
</tr>
<tr>
<td>PH₃+hν → PH₂+H</td>
<td>See table notes</td>
<td>(10)</td>
</tr>
</tbody>
</table>

Notes. Bi-molecular reaction coefficients are shown in cm³ s⁻¹ and termolecular reactions are in cm³ s⁻¹. The unit of temperature, T, is K and the unit of number density, N, is cm⁻³. All reactions are valid for temperatures around 298 K. Photolysis cross sections are taken from Chen et al. (1991) between 120 and 230 nm. The quantum yield is assumed to be unity.

References. (1) Nava & Stief (1989); (2) Fritz et al. (1982); (3) Wang et al. (2005); (4) Arthur & Cooper (1997); (5) Iyer et al. (1983); (6) Hamilton & Murrells (1985); (7) Bosco et al. (1983); (8) Kaye & Strobel (1984); (9) rate assumed to be the same as the reaction P₄+P₄+M→P₃+M; (10) Chen et al. (1991).

### Table 2. Climate-only scenarios: surface pressure range (p₀, in bar) and mixing ratios (f) of N₂, CO₂, H₂, and He considered for LHS 1140 b.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>p₀</th>
<th>N₂</th>
<th>CO₂</th>
<th>H₂</th>
<th>He</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>0.7–100</td>
<td>0.9996</td>
<td>4 × 10⁻⁴</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>II</td>
<td>0.1–22</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>III</td>
<td>0.1–6</td>
<td>0</td>
<td>0</td>
<td>0.8</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Environmental conditions LHS 1140 b could be habitable at the surface (see Table 2). The mixing ratios of the species are constant over height. We consider pressures leading to surface temperatures between 220 K (approximated limit of open water with ocean heat transport in climates of tidally locked exoplanets around M dwarf stars; see Hu & Yang 2014; Checlair et al. 2017, 2019) and 395 K (see Clarke 2004; McKay 2014). In addition, we limit our calculation to 100 bar surface pressure since massive envelopes are not expected due to the high bulk density of the planet (Ment et al. 2019).

We include absorption by the major radiative species (Scheucher et al. 2020). For the H₂O profile we use a constant relative humidity of 80% up to the tropopause. Above the tropopause the H₂O profile is set to a constant abundance based on its value at the cold trap. For the N₂ atmospheres we assume an Earth-like CO₂ level of 400 ppm (see, e.g., Monastersky 2013) and for the H₂-dominated atmospheres we use 80% H₂ and 20% He.

2.3. Climate-only runs

We perform climate-only runs of N₂-dominated, CO₂, and H₂–He atmospheres with the radiative transfer module REDFOX, and vary the surface pressures in order to investigate for which atmospheric conditions LHS 1140 b could be habitable at the surface (see Table 2). The mixing ratios of the species are constant over height. We consider pressures leading to surface temperatures between 220 K (approximated limit of open water with ocean heat transport in climates of tidally locked exoplanets around M dwarf stars; see Hu & Yang 2014; Checlair et al. 2017, 2019) and 395 K (see Clarke 2004; McKay 2014). In addition, we limit our calculation to 100 bar surface pressure since massive envelopes are not expected due to the high bulk density of the planet (Ment et al. 2019).

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Table 3. Climate–chemistry scenarios: surface mixing ratio of CO$_2$, H$_2$, He, and CH$_4$.

<table>
<thead>
<tr>
<th>Scenario</th>
<th>CO$_2$</th>
<th>H$_2$</th>
<th>He</th>
<th>CH$_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>1 × 10^{-9}</td>
<td>Fill gas</td>
<td>0.2</td>
<td>1 × 10^{-6}</td>
</tr>
<tr>
<td>1b</td>
<td>1 × 10^{-3}</td>
<td>Fill gas</td>
<td>0.198</td>
<td>1 × 10^{-3}</td>
</tr>
<tr>
<td>1c</td>
<td>0.01</td>
<td>Fill gas</td>
<td>0.18</td>
<td>1 × 10^{-3}</td>
</tr>
<tr>
<td>2a</td>
<td>1 × 10^{-6}</td>
<td>Fill gas</td>
<td>0.14</td>
<td>1 × 10^{-3}</td>
</tr>
<tr>
<td>2b</td>
<td>0.1</td>
<td>Fill gas</td>
<td>0.06</td>
<td>1 × 10^{-3}</td>
</tr>
<tr>
<td>2c</td>
<td>0.4</td>
<td>Fill gas</td>
<td>0.02</td>
<td>1 × 10^{-3}</td>
</tr>
<tr>
<td>3a</td>
<td>8 × 10^{-3}</td>
<td>Fill gas</td>
<td>2 × 10^{-3}</td>
<td>1 × 10^{-3}</td>
</tr>
<tr>
<td>3b</td>
<td>8 × 10^{-6}</td>
<td>Fill gas</td>
<td>2 × 10^{-6}</td>
<td>1 × 10^{-3}</td>
</tr>
</tbody>
</table>

Notes. Fill gas denotes the main constituent of the atmosphere. Scenario 1c has a composition similar to Neptune: an H$_2$-dominated atmosphere with 20% He (Williams et al. 2004), 1 ppb CO$_2$ (Meadows et al. 2008), and 3% CH$_4$ (Irwin et al. 2019). Scenario 10a has a CO$_2$-dominated atmosphere with ∼10 ppm H$_2$ and He similar to Mars and Venus (Krasnopolsky & Gladstone 2005; Krasnopolsky & Feldman 2001). For each of the ten main scenarios regarding the main composition of the atmosphere we consider three different boundary conditions of CH$_4$ (see text).

2.4. Coupled climate–chemistry runs

Here we apply the coupled version of 1D-TERRA to simulate the potential atmospheric temperature and composition profiles of LHS 1140 b. All simulations assume a constant relative humidity of 80% from the surface to the cold trap. The surface albedo is set to 0.255, which is the value needed to achieve a mean surface temperature of 288.15 K for the Earth around the Sun (see Scheucher et al. 2020; Wunderlich et al. 2020).

Table 3 shows the 30 scenarios performed with the coupled-climate model. All scenarios assume a constant surface pressure of 2.416 bar, corresponding to the atmospheric pressure of the Earth assuming a surface gravity $g$ of 23.7 m s$^{-2}$ for LHS 1140 b (Ment et al. 2019). We chose this moderate surface pressure for the following reasons. LHS 1140 b has a high bulk density ($\rho$) of 7.5 ± 1.0 cm$^{-3}$ (Ment et al. 2019). Hence, it is unlikely that the planet has a thick H$_2$ or He envelope. However, the enhanced gravity compared to Earth results in reduced H$_2$ escape rates (see, e.g., Pierrehumbert & Gaidos 2011). This is supported by theoretical studies showing that cool and/or massive super-Earths can retain small residual H$_2$–He envelopes at the end of the core-powered mass loss (Misener & Schlichting, in prep.; Gupta & Schlichting 2019; Ginzburg et al. 2016). The secondary outgassing of CO$_2$ is expected to be small for a super-Earth like LHS 1140 b with a mass of ∼7 $M_{\oplus}$ (see, e.g., Dorn et al. 2018; Noack et al. 2017). Hence, we do not consider thick CO$_2$ atmospheres as on Venus.

In this study we vary the atmospheric mixtures of H$_2$–He and CO$_2$ in ten steps (see Table 3). For each of the steps we also consider three different boundary conditions for CH$_4$. The CH$_4$ abundance can have a large impact on surface temperature and habitability (see, e.g., Pavlov et al. 2000; Ramirez & Kaltenegger 2018). The detectability of atmospheric spectral features on exoplanets can also largely depend on the CH$_4$ inventory due to haze formation or CH$_4$ absorption (see, e.g., Arney et al. 2016, 2017; Lavvas et al. 2019; Wunderlich et al. 2019). We vary the boundary conditions of CH$_4$ as follows:

a: The “low CH$_4$” scenarios assume the volume mixing ratio (vmr) of CH$_4$ to be constant at 1 × 10^{-6} at the surface, corresponding roughly to the surface CH$_4$ concentration in the pre-industrial era on Earth (see, e.g., Etheridge et al. 1998).
b: The “medium CH$_4$” scenarios use a constant CH$_4$ vmr of 1 × 10^{-3} at the surface. Model studies such as Rugheimer et al. (2015) and Wunderlich et al. (2019) suggest a CH$_4$ vmr of roughly 1 × 10^{-3} for Earth-like planets in the HZ around mid-M dwarfs using a surface emission of 1.4 × 10^{11} molec. cm$^{-2}$ s$^{-1}$, as measured on Earth (e.g., Lelieveld et al. 1998).
c: The “high CH$_4$” scenarios assume that the surface vmr of CH$_4$ is constant at 3%. This is consistent with the observed main composition of the lower atmosphere of Neptune with 2–4% CH$_4$ at 2 bar (see, e.g., Irwin et al. 2019).

We assume the same boundaries for all 30 scenarios (except for CO$_2$, H$_2$, He, and CH$_4$). For O$_2$, CO, H$_2$S, NO, N$_2$, OCS, HCN, C$_2$S, CH$_3$OH, C$_2$H$_6$, H$_2$S, and HCl we assume pre-industrial Earth-like biogenic fluxes (see Table 4). Regarding NH$_3$, PH$_3$, and CH$_3$Cl we use higher biogenic fluxes than measured on Earth, assuming that an H$_2$-dominated atmosphere could favor the biogenic production of these species, since H$_2$ can act as a nutrient. We assume a biogenic NH$_3$ flux of 8.38 × 10^{10} molecules cm$^{-2}$ s$^{-1}$ corresponding to mean global emissions on a hypothetical cold Haber world (Seager et al. 2013a). This NH$_3$ flux is ∼100 times higher than that observed on pre-industrial Earth (Bouwman et al. 1997). The assumed biogenic emissions of CH$_3$Cl are assumed to be 100 times greater than on pre-industrial Earth (Seinfeld & Pandis 2016). The biogenic surface flux of PH$_3$ is taken from Sousa-Silva et al. (2020). Additionally, we apply biogenic and volcanic emissions as measured on Earth (see Table 4 and Wunderlich et al. 2020, for references). We assume a non-zero dry deposition velocity ($v_{dep}$) for all species to reduce a potential runaway effect (see, e.g., Hu et al. 2020). For CH$_4$, O$_2$, CH$_3$Cl, PH$_3$, NH$_3$, and N$_2$O we assume a $v_{dep}$ of 1 × 10^{-8} cm s$^{-1}$. For O$_2$ this value was used by other model studies (e.g., Arney et al. 2016; Hu et al. 2020; Wunderlich et al. 2020) and provides an upper estimation of how much of these gases could be accumulated for the scenarios assumed. For all other species we use a $v_{dep}$ of 0.02 cm s$^{-1}$, following Hu et al. (2012) and Zahnle et al. (2008).
2.5. Transmission

The simulated atmospheres serve as input to compute transmission spectra with the Generic Atmospheric Radiation Line-by-line Infrared Code (GARLIC; Schreier et al. 2014, 2018). Line parameters and CIAs are taken from the HITRAN database (Gordon et al. 2017; Karman et al. 2019). We consider the CKD continuum model for H$_2$O (Clough et al. 1989) and Rayleigh extinction for H$_2$, He, CO$_2$, H$_2$O, N$_2$, CH$_4$, CO, N$_2$O, and O$_2$ (Murphy 1977; Sneep & Ubachs 2005; Marcq et al. 2011). In the visible we use the cross sections at room temperature (298 K) listed in Table 3 of Wunderlich et al. (2020).

We assume cloud-free conditions for all simulated transmission spectra. We do, however, consider extinction from uniformly distributed aerosols with an optical depth ($\tau_A$) at wavelength $\lambda$ (µm) following Ångström (1930), Allen (1976), and Yan et al. (2015):

$$\tau_A = \beta \cdot N_c \cdot \lambda^{-\alpha},$$  

(1)

with the column density ($N_c$) in molecules cm$^{-2}$. For clear sky conditions with weak scattering by haze or dust we set $\alpha$ to 1.3, representing an average measured value on Earth following the Junge distribution (see, e.g., Ångström 1961) and we set the coefficient $\beta$ to $1.4 \times 10^{-27}$ following Allen (1976). For hazy conditions we assume $\alpha$ to be 2.6 and set $\beta$ to $6.0 \times 10^{-25}$, representing the best fit to extinction by hazes on Titan (see Appendix C). It should be noted that we do not consider the production of hazes in H$_2$- and CO$_2$-dominated atmospheres in our model. The assumed impact of hazes on the spectral appearance of the simulated atmospheres should therefore only serve as a rough estimation, and further investigation is needed to test the validity of this assumption.

We express the transmission spectra as wavelength-dependent atmospheric transit depth, which contains the contribution of the atmosphere to the total transit depth without the contribution from the solid body (see more details in Schreier et al. 2018; Wunderlich et al. 2020).

<table>
<thead>
<tr>
<th>Species</th>
<th>Emissions (molec. cm$^{-2}$ s$^{-1}$)</th>
<th>$\nu_{dep}$ (cm s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O$_2$</td>
<td>$1.21 \times 10^{12}$</td>
<td>$1 \times 10^{-8}$</td>
</tr>
<tr>
<td>CH$_3$Cl</td>
<td>$1.39 \times 10^{10}$</td>
<td>$1 \times 10^{-8}$</td>
</tr>
<tr>
<td>PH$_3$</td>
<td>$1.00 \times 10^{10}$</td>
<td>$1 \times 10^{-8}$</td>
</tr>
<tr>
<td>NH$_3$</td>
<td>$8.38 \times 10^{10}$</td>
<td>$1 \times 10^{-8}$</td>
</tr>
<tr>
<td>N$_2$O</td>
<td>$7.80 \times 10^6$</td>
<td>$1 \times 10^{-8}$</td>
</tr>
<tr>
<td>CO</td>
<td>$1.07 \times 10^{11}$</td>
<td>0.02</td>
</tr>
<tr>
<td>NO</td>
<td>$3.38 \times 10^6$</td>
<td>0.02</td>
</tr>
<tr>
<td>H$_2$S</td>
<td>$3.73 \times 10^6$</td>
<td>0.02</td>
</tr>
<tr>
<td>SO$_2$</td>
<td>$1.34 \times 10^{10}$</td>
<td>0.02</td>
</tr>
<tr>
<td>OCS</td>
<td>$1.42 \times 10^6$</td>
<td>0.02</td>
</tr>
<tr>
<td>HCN</td>
<td>$1.27 \times 10^7$</td>
<td>0.02</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>$3.35 \times 10^{10}$</td>
<td>0.02</td>
</tr>
<tr>
<td>CS$_2$</td>
<td>$5.05 \times 10^8$</td>
<td>0.02</td>
</tr>
<tr>
<td>C$_2$H$_6$</td>
<td>$8.55 \times 10^6$</td>
<td>0.02</td>
</tr>
<tr>
<td>C$_3$H$_8$</td>
<td>$9.51 \times 10^6$</td>
<td>0.02</td>
</tr>
<tr>
<td>HCl</td>
<td>$5.57 \times 10^6$</td>
<td>0.02</td>
</tr>
</tbody>
</table>

2.6. Signal-to-noise ratio (S/N)

An important aim of this study is to determine whether molecular absorption features are detectable with the JWST and ELT (see Table 5). For low-resolution spectroscopy (LRS) we calculate the required number of transits with JWST NIRSpec PRISM and MIRI LRS with the method presented in Wunderlich et al. (2019). LHS 1140 exceeds the brightness limits of NIRSpec PRISM leading to a saturation of the detector between 1 and 2 µm. Hence, we consider partial saturation of the detector, as proposed by Batalla et al. (2018), and exclude the wavelength range between 1 and 2 µm from our analysis. The results do not significantly differ when we use medium-resolution filters such as NIRSpec G235M and G395M (Birkmann et al. 2016), which do not saturate for LHS 1140. However, the two filters cannot be used simultaneously because it would decrease the wavelength coverage compared to NIRSpec PRISM, and the additional binning of the spectral data with higher resolving power might lead to enhanced red noise.

With high-resolution spectroscopy (HRS) we investigated the potential detection of spectral lines from NH$_3$, PH$_3$, CH$_3$Cl, and N$_2$O with the cross-correlation technique using the HIRES and METIS instruments on ELT. We used the same approach to estimate the number of transits necessary to detect the molecules with the cross-correlation method, as described in Wunderlich et al. (2020). The S/N of the star per transit is calculated with the European Southern Observatory Exposure Time Calculator (ESO ETC) Version 6.4.0 from November 2019 (see updated documentation$^4$ from Liske 2008). As input for the ETC we use the stellar spectrum described in Sect. 2.1 and scale it to the $K$-band magnitude of 8.821 (Cutri et al. 2003) in order to obtain the input flux distribution. Equivalent to Wunderlich et al. (2020) we used a mean throughput of 10% for ELT HIRES and METIS. Previous studies investigating the feasibility of detection of O$_2$, for example, in Earth-like atmospheres assumed a more optimistic throughput of 20% (Snellen et al. 2013; Rodler & López-Morales 2014; Serindag & Snellen 2019). The sky conditions are set to a constant airmass of 1.5 and a precipitable water vapor (PWV) of 2.5. For each wavelength band we changed the radius of the diffraction limited core of the point spread function according to the recommendation in Liske (2008).

Table 5. Wavelength coverage and resolving power ($R$) of the instruments on JWST and ELT used to calculate the number of transits required to detect spectral features in the atmosphere of LHS 1140 b.

<table>
<thead>
<tr>
<th>Telescope - Instrument</th>
<th>Wavelength</th>
<th>$R$</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>JWST - NIRSpec PRISM</td>
<td>0.6–5.3 µm</td>
<td>~100</td>
<td>(1)</td>
</tr>
<tr>
<td>JWST - MIRI LRS</td>
<td>5.0–12 µm</td>
<td>~100</td>
<td>(2)</td>
</tr>
<tr>
<td>ELT - HIRES</td>
<td>0.37–2.5 µm</td>
<td>100000</td>
<td>(3)</td>
</tr>
<tr>
<td>ELT - METIS (HRS)</td>
<td>2.9–5.3 µm</td>
<td>100000</td>
<td>(4)</td>
</tr>
</tbody>
</table>

References. (1) Birkmann et al. (2016); (2) Kendrew et al. (2015); (3) Marconi et al. (2016); (4) Brandl et al. (2016).

3 https://www.eso.org/observing/etc/bin/gen/form?INS.NAME=ELT+INS.MODE=swspectr
4 https://www.eso.org/observing/etc/doc/elt/etc_spec_model.pdf
3. Results and discussion

3.1. Surface habitability

Figure 1 shows the surface temperatures of LHS 1140 b for N$_2$-, CO$_2$-, and H$_2$-dominated atmospheres with varying surface pressures, for the climate-only runs (without coupling to the photochemistry module, see Sect. 2.3). The results suggest that thick N$_2$-dominated atmosphere on LHS-1140 b or substantial amounts of greenhouse gases such as CO$_2$ are required to reach habitable surface temperatures. The simulations show that a CO$_2$ atmosphere requires a surface pressure of $\sim$2.5 bar to reach a global mean surface temperature above 273 K. This is comparable to the results of Morley et al. (2017) who found that a 2 bar Venus-like atmosphere on LHS 1140 b would lead to a surface temperature of around 280 K.

For an H$_2$ atmosphere, the atmosphere extends the outer edge of the HZ (see, e.g., Pierrehumbert & Gaidos 2011) compared to CO$_2$ atmospheres. The simulated H$_2$ atmospheres have up to 80 K warmer surface temperatures than the CO$_2$ atmospheres. Our results suggest that a surface pressure of 0.6 bar leads to a surface temperature of about 273 K on LHS 1140 b.

3.2. Atmospheric profiles

To simulate the atmospheric scenarios as described in Sect. 2.4 we use the coupled version of 1D-TERRA. Figure 2 shows the temperature and composition profiles of selected species for H$_2$-dominated atmospheres with low concentrations of CO$_2$ (scenarios 1a, 1b, and 1c; see Sect. 2.4 and Table 3) and CO$_2$-dominated atmospheres with low concentrations of H$_2$ (scenarios 10a, 10b, and 10c). Figure 3 shows the surface temperature, the atmospheric height at the top of atmosphere (ToA) at $\sim$0.01 Pa, the surface vmr of CO$_2$, H$_2$O, and O$_2$, and the CH$_4$ vmr at the ToA with decreasing concentrations of H$_2$ (corresponding to increasing concentrations of CO$_2$; see Table 3).

3.2.1. Temperature

Figure 2 suggests that the H$_2$-dominated atmospheres with low and medium CH$_4$ concentrations (corresponding to scenarios 1a and 1b, respectively) show a similar temperature profile from the surface up to $\sim$200 hPa with a strong warming towards the ToA. The H$_2$-dominated atmosphere with a high CH$_4$ concentration (scenario 1c) results in a warm stratosphere due to CH$_4$ short-wave absorption and accordingly a cool troposphere, similar to the shape of the temperature profile behavior on Titan (see, e.g., Fulchignoni et al. 2005; Serigano et al. 2016). The high concentration of CH$_4$ absorbs most of the stellar energy in the stratosphere, leading to reduced stellar irradiation reaching the troposphere (see also Ramirez & Kaltenegger 2018). We note that 1D-TERRA does not consider the effect of hazes that might be formed in such an environment (see, e.g., He et al. 2018; Hörst et al. 2018).

In CO$_2$-dominated atmospheres we simulate similar temperature profiles for low CH$_4$ concentrations (scenario 10a) compared to medium CH$_4$ concentrations (scenario 10b). There is no temperature inversion from O$_3$ absorption in the middle atmosphere due to the weak UV emission of M dwarfs (see also, e.g., Segura et al. 2005; Grenfell et al. 2014; Wunderlich et al. 2019, 2020). The CO$_2$-dominated atmosphere with high abundances of CH$_4$ (scenario 10c) shows weak temperature variations in the range of $\sim$40 K through the simulated atmospheric profile. The high concentration of CH$_4$ leads to a warming of the atmosphere compared to the runs with lower CH$_4$ abundances, except near the surface, where the anti-greenhouse effect cools the atmosphere.

In Fig. 3 the low and medium CH$_4$ scenarios (blue and green lines, respectively) feature similar responses in surface temperatures with decreasing H$_2$. The high CH$_4$ scenarios (orange line) first show a warming effect of about 50 K due to the decreased partial pressure of CH$_4$ with increasing molecular weight towards CO$_2$-rich atmospheres (scenarios 1c to 4c). We note that the surface mixing ratio of CH$_4$ is kept constant at 3% for all the high CH$_4$ scenarios. For CO$_2$-dominated atmospheres the surface temperature decreases when reducing the abundances of H$_2$ (scenarios 6c to 10c) due to the weaker warming from the H$_2$-H$_2$ CIA.

3.2.2. H$_2$O

The water profile in the lower atmosphere depends mainly on the assumed relative humidity and the temperature profile near the surface. For all simulations we assume the relative humidity to be constant at 80% up to the tropopause. In the middle and upper atmosphere the H$_2$O profile is determined mainly by chemical production or loss and to a lesser extent by eddy mixing. H$_2$O is mainly destroyed by photolysis at wavelengths below 200 nm forming the hydroxyl radical (OH) and atomic hydrogen (H):

$$\text{H}_2\text{O} + h\nu \rightarrow \text{H} + \text{OH}.$$  \hspace{1cm} (R1)

The H$_2$-dominated atmospheres show weaker FUV absorption compared to the CO$_2$-dominated atmospheres. This weaker shielding effect leads to enhanced photolysis and less stratospheric water content for the scenarios with H$_2$-dominated atmospheres (Fig. 2). For the high CH$_4$ scenarios the water photolysis is weak due to strong FUV absorption from CH$_4$. In CO$_2$-dominated atmospheres H$_2$O is significantly reformed via H$_2$O$_2$-driven (HO$_2$ + H + OH + HO$_2$) oxidation of CH$_4$ at pressures less than 0.1 hPa (see also Segura et al. 2005; Grenfell et al. 2013; Rugheimer et al. 2015; Wunderlich et al. 2019).

3.2.3. O$_2$

All runs assume an Earth-like surface O$_2$ flux from photosynthesis (see Table 4). However, in H$_2$-dominated atmospheres the oxygen content near the surface is only $\sim$1 ppm for low and medium CH$_4$ scenarios (blue and green solid line in Fig. 2). Grenfell et al. (2018) suggest that the catalytic cycles including HO$_2$ and NO$_x$ leads to oxidation of H$_2$ into water. O$_2$ is mainly
Fig. 2. Simulated temperature and composition profiles of selected species of LHS 1140 b. Different colors represent the three types of scenarios considered: blue for low CH$_4$, green for medium CH$_4$, and orange for high CH$_4$. The solid lines represent H$_2$-dominated atmospheres (scenarios 1a, 1b, and 1c), whereas the dashed lines show CO$_2$-dominated atmospheres (scenarios 10a, 10b, 10c).

destroyed via photolysis or the three-body reaction with atomic hydrogen:

$$\text{O}_2 + h\nu \rightarrow \text{O} + \text{O}, \quad \text{(R2)}$$

$$\text{H} + \text{O}_2 + \text{M} \rightarrow \text{HO}_2 + \text{M}. \quad \text{(R3)}$$

The atomic hydrogen required for reaction (R3) is mainly produced via

$$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}. \quad \text{(R4)}$$

OH can be formed via the reactions

$$\text{H} + \text{HO}_2 \rightarrow \text{OH} + \text{OH}, \quad \text{(R5)}$$

$$\text{H} + \text{NO}_2 \rightarrow \text{OH} + \text{NO}, \quad \text{(R6)}$$

$$\text{HO}_2 + \text{NO} \rightarrow \text{OH} + \text{NO}_2, \quad \text{(R7)}$$

and by water photolysis (reaction (R1)), which increases the concentration of H in the middle atmosphere. The atomic hydrogen can be removed via escape or it can recombine to form H$_2$ (see Hu et al. 2012). For the H$_2$-dominated atmosphere with high CH$_4$ concentrations (scenario 1c) the surface mixing ratio of O$_2$ is two orders of magnitudes higher than for scenarios 1a and 1b due to the lower concentrations of NO$_x$ and H in the lower atmosphere.

For increasing mixing ratios of CO$_2$ the destruction of O$_2$ via H$_2$ oxidation is less dominant, and O$_2$ can accumulate in

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the atmosphere (see Fig. 3). The CO$_2$-dominated atmospheres with less than 10% H$_2$ feature high abundances of O$_2$ of up to 30% for the atmospheres with low and medium CH$_4$ concentrations (scenario 8a–10a and 8b–10b). For scenarios 8a and 8b the concentration of O$_2$ might be limited to about 10% (see gray shaded region in Fig. 3) due to the potential combustion of the atmosphere (Grenfell et al. 2018).

The high concentrations of O$_2$ are related to the lower UV flux of M dwarfs (hence weaker O$_3$ photolysis) as well as strong abiotic production of O$_2$ from CO$_2$ photolysis at wavelengths below 200 nm (see also, e.g., Domagal-Goldman et al. 2014; Harman et al. 2015; Wunderlich et al. 2020). The lower FUV/NUV value of LHS 1140 compared to a solar-type star (see, e.g., Brasseur & Solomon 2006). The main O$_3$ sinks are photolysis at wavelengths less than ~200 nm and catalytic cycles involving HO$_x$ and NO$_x$, which convert O$_3$ into O$_2$ in the middle atmosphere (see, e.g., Brasseur & Solomon 2006; Grenfell et al. 2013).

In our scenarios the low FUV/NUV environment compared with the Earth favors weak release of HO$_x$ and NO$_x$ from their reservoir molecules, which leads to weak O$_3$ catalytic loss. The low and medium CH$_4$ scenarios with CO$_2$-dominated atmospheres show an ozone layer with peak abundances (~20–50 ppm) up to about five times higher than on Earth (compare to Fig. 2 in Wunderlich et al. 2020). Grenfell et al. (2014) suggest that the smog mechanism is an important O$_3$ source for late M dwarfs since UV levels are not sufficient to efficiently drive the Chapman mechanism. All scenarios with H$_2$O-dominated atmospheres and CO$_2$-dominated atmosphere with high concentrations of CH$_4$ are however low in O$_2$, leading overall to weak production of O$_3$.

3.2.5. CO

All simulations assume emissions of CO from volcanoes and biomass based on pre-industrial Earth values. An important in situ sink for CO is OH via

\[ \text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}. \]  (R16)

The production of O$_2$ is further enhanced by the presence of OH via

\[ \text{O} + \text{OH} \rightarrow \text{O}_2 + \text{H}. \]  (R10)

CO and O can recombine to CO$_2$ via a HO$_x$ catalyzed reaction sequence, forming CO$_2$: CO + O $\rightarrow$ CO$_2$ (see, e.g., Domagal-Goldman et al. 2014; Gao et al. 2015; Meadows 2017; Schwieterman et al. 2019). For the CO$_2$-dominated atmosphere with high CH$_4$ concentrations we find that atomic oxygen (O) quickly reacts with CH$_3$ via

\[ \text{O} + \text{CH}_3 \rightarrow \text{H}_2\text{CO} + \text{H}. \]  (R11)

or

\[ \text{O} + \text{CH}_3 \rightarrow \text{CO} + \text{H}_2 + \text{H}. \]  (R12)

forming H$_2$, H, CO, and H$_2$CO. Part of the H$_2$CO separates into H$_2$ and CO via

\[ \text{H}_2\text{CO} + \nu \rightarrow \text{H}_2 + \text{CO} \]  (R13)

or

\[ \text{H}_2\text{CO} + \text{H} \rightarrow \text{H}_2 + \text{HCO} \]  (R14)

\[ \text{HCO} + \text{H} \rightarrow \text{H}_2 + \text{CO}. \]  (R15)

Hence, the results suggest low concentrations of O$_2$ and high abundances of CO for the high CH$_4$ scenarios with CO$_2$-dominated atmospheres.

3.2.4. O$_3$

A main source of O$_3$ largely depends on the amount of O$_3$ available for photolysis in the atmosphere. O$_3$ is split into atomic oxygen via photolysis between 170 and 240 nm (reaction (R2)) and then reacts with O$_3$ to form O$_3$ via a fast three-body reaction (see, e.g., Brasseur & Solomon 2006). The main O$_3$ sinks are photolysis at wavelengths less than ~200 nm and catalytic cycles involving HO$_x$ and NO$_x$, which convert O$_3$ into O$_2$ in the middle atmosphere (see, e.g., Brasseur & Solomon 2006; Grenfell et al. 2013).

Fig. 3. Change in surface temperature in K; in atmospheric height at ToA (~0.01 Pa) in km; and in surface volume mixing ratio (vmr) of H$_2$O, CO, and CH$_4$ with decreasing concentrations of H$_2$ for scenarios with low (blue lines), medium (green lines), and high CH$_4$ scenarios. The concentrations of CO$_2$ corresponding to H$_2$ vmrs of 0.75, 0.5, 0.25, and 0.0 are shown in green on the top x-axis for the medium CH$_4$ scenarios. The colored dots represent the ten individual main scenarios described in Table 3. The dashed black line shows $T = 273$ K. The gray shaded region represents the limits of combustion for H$_2$-CO$_2$ and H$_2$-O$_2$ gas mixtures (see Grenfell et al. 2018). The assumed surface mixing ratios of H$_2$ and CO$_2$ for the main scenarios 5–8 are at the edge of the H$_2$-CO$_2$ combustion limit.

2(CO$_2$ + h$v$ $\rightarrow$ CO + O) \hspace{1cm} \text{(R8)}

O + O + M $\rightarrow$ O$_2$ + M \hspace{1cm} \text{(R9)}

2CO$_2$ $\rightarrow$ 2CO + O$_2$
Our results suggest a decreased OH due to a slowing of its main source reaction,

\[ \text{O}_3^+ + \text{H}_2 \rightarrow 2\text{OH}, \quad (R17) \]

since production of \( \text{O}_3^+ \) (e.g., from \( \text{O}_3 \) photolysis) is disfavored by the stellar UV emission. The weak OH favors an increase in CO and \( \text{CH}_4 \) by several orders of magnitude compared with modern Earth. Similar effects have been noted by several studies in the literature for Earth-like planets (see, e.g., Segura et al. 2005; Grenfell et al. 2007; Rugheimer et al. 2015; Wunderlich et al. 2019).

The tropospheric temperature of the \( \text{H}_2 \)-dominated atmosphere with high concentrations of \( \text{CH}_4 \) (scenario 1c) is much lower compared to the other scenarios due to the strong \( \text{CH}_4 \) anti-greenhouse effect (see above), leading to water condensation and hence less water photolysis in the troposphere. We note that the OH radical can also be formed via \( \text{HO}_2 \) re-partitioning (reaction (R7)), which can be driven by enhancements in NO via incoming cosmic rays (see, e.g., Airapetian et al. 2016, 2020; Scheucher et al. 2018).

In the atmosphere with high concentrations of \( \text{CH}_4 \) results suggest that the recombination of CO and O into \( \text{CO}_2 \) is weakened due to the additional sinks of atomic oxygen via reactions (R11) and (R12) as discussed in Sect. 3.2.3. High \( \text{CH}_4 \) generally favors lowered OH, which weakens the HO\(_2\) catalyzed combination of CO and O into \( \text{CO}_2 \). This leads to higher abundances of CO for high \( \text{CH}_4 \) scenarios compared to the other scenarios.

### 3.2.6. \( \text{CH}_4 \) and hydrocarbons

Understanding how \( \text{CH}_4 \) forms higher-order hydrocarbons (\( \text{C}_n \)) and how these species are subsequently removed to reform \( \text{CH}_4 \) is a central issue because higher-order hydrocarbons can readily condense to form hazes, which could strongly impact climate and observed spectra. The high \( \text{CH}_4 \) scenarios feature a large production of hydrocarbons such as \( \text{C}_2\text{H}_2 \), \( \text{C}_2\text{H}_4 \), and \( \text{C}_2\text{H}_6 \). Figure 2 shows the atmospheric profiles of \( \text{C}_2\text{H}_6 \), but we note that \( \text{C}_2\text{H}_2 \) and \( \text{C}_2\text{H}_4 \) (not shown) have concentrations similar to \( \text{C}_2\text{H}_6 \) with the highest mixing ratios of up to 0.1% at the TOA.

Our results suggest that in \( \text{H}_2 \)-dominated atmospheres the main pathway for initiating ascent of the homologous chain from \( \text{C}_1 \rightarrow \text{C}_2 \) (\( \text{CH}_4 \rightarrow \text{C}_2\text{H}_6 \)) pathway is as follows:

\[
\begin{align*}
2(\text{CH}_4 + \nu & \rightarrow 1\text{CH}_2 + \text{H}_2) \quad (R18) \\
2(1\text{CH}_2 + \text{H}_2 & \rightarrow \text{CH}_3 + \text{H}) \quad (R19) \\
\text{CH}_3 + \text{CH}_3 + \text{M} & \rightarrow \text{C}_2\text{H}_6 + \text{M} \quad (R20)
\end{align*}
\]

\( \text{2CH}_4 \rightarrow \text{C}_2\text{H}_6 + 2\text{H}. \)

The above pathway is an established route for ascending the hydrocarbon chain (see, e.g., Yung & DeMore 1999, Chapter 5 and references therein). It is initiated by \( \text{CH}_4 \) photolysis to form reactive methyl radicals (\( \text{CH}_3 \)), which participate in a three-body self-reaction to form ethane (\( \text{C}_2\text{H}_6 \)).

Our results suggest that \( \text{C}_2\text{H}_4 \) is mainly formed by the reactions

\[
\begin{align*}
\text{CH} + \text{CH}_4 & \rightarrow \text{C}_2\text{H}_4 + \text{H} \quad (R21) \\
\text{CH}_2 + \text{CH}_3 & \rightarrow \text{C}_2\text{H}_4 + \text{H}, \quad (R22)
\end{align*}
\]

where \( \text{CH} \) is produced via

\[
\begin{align*}
\text{CH}_4 + \nu & \rightarrow \text{CH} + \text{H}_2 + \text{H} \quad (R23) \\
\text{CH}_3 + \nu & \rightarrow \text{CH} + \text{H}_2 \quad (R24) \\
\text{H} + \text{CH}_2 & \rightarrow \text{CH} + \text{H}_2, \quad (R25)
\end{align*}
\]

and \( \text{C}_2\text{H}_2 \) is formed via photolysis of \( \text{C}_2\text{H}_4 \) and the reaction

\[
\text{CH}_2 + \text{CH}_2 \rightarrow \text{C}_2\text{H}_2 + \text{H}_2 \quad (R26)
\]

(see also Yung & DeMore 1999, and references therein).

In \( \text{CO}_2 \)-dominated atmospheres our results suggest that the reaction (R19) is slower due to reduced \( \text{H}_2 \), and because part of the \( \text{CH}_2 \) reacts with \( \text{CO}_2 \) forming \( \text{H}_2\text{CO} \) and \( \text{CO} \). This effect disfavors the pathway producing \( \text{C}_2\text{H}_6 \). Additionally, however, the destruction of \( \text{CH}_3 \) via

\[
\text{CH}_3 + \text{H}_2 \rightarrow \text{CH}_4 + \text{H} \quad (R27)
\]

is weakened due to lowered \( \text{H}_2 \). This effect favors enhanced \( \text{CH}_3 \), hence the pathway producing \( \text{C}_2\text{H}_6 \). The overall effect is slightly lower concentrations of \( \text{CH}_4 \) in the upper atmosphere but larger amounts of \( \text{C}_2\text{H}_6 \) as well as \( \text{C}_2\text{H}_2 \) and \( \text{C}_2\text{H}_4 \) (not shown) for \( \text{CO}_2 \)-dominated atmospheres compared to \( \text{H}_2 \)-dominated atmospheres when assuming high concentrations of \( \text{CH}_4 \).

The higher abundances of \( \text{C}_2\text{H}_2 \) shown in Figs. 2 and 3 for scenario 10c compared to scenario 1c suggests more haze production by hydrocarbons in \( \text{CO}_2 \)-dominated compared with \( \text{H}_2 \)-dominated atmospheres. This effect would be reinforced assuming \( \text{CO}_2 \)-dominated atmospheres have cooler mid to upper atmospheres compared with \( \text{H}_2 \)-dominated atmospheres, as suggested by Fig. 2. We note, however, that the above result could be reversed in atmospheres where \( \text{CH}_2 \) (reaction (R19)) becomes more important for \( \text{C}_2\text{H}_6 \) production since \( \text{H}_2 \)-dominated atmospheres favor reduced \( \text{CH}_2 \), as discussed above. For the low and medium \( \text{CH}_4 \) scenarios the concentrations of \( \text{C}_2\text{H}_4 \) decrease with decreasing \( \text{CH}_4/\text{CO}_2 \) values, as suggested by Arney et al. (2018), among others, for \( \text{N}_2 \)-dominated atmospheres.

### 3.2.7. \( \text{SO}_2 \)

We assume volcanic outgassing of \( \text{SO}_2 \) as measured on modern Earth. Due to its high solubility in water-forming sulfate, \( \text{SO}_2 \) is deposited easily over wet surfaces leading to \( \text{SO}_2 \) surface mixing ratios below 1 ppb. The main in situ chemical sink of \( \text{SO}_2 \) is photodissociation below 400 nm (e.g., Manatt & Lane 1993), and its oxidation via reaction with \( \text{OH} \) or \( \text{O}_3 \) to ultimately form \( \text{SO}_3 \), which quickly reacts with water to form sulfate (see, e.g., Burkholder et al. 2015; Seinfeld & Pandis 2016). In \( \text{CO}_2 \)-dominated atmospheres with low and medium \( \text{CH}_4 \) concentrations (scenarios 10a and 10b), the results suggest that shielding associated with high UV absorption from \( \text{CO}_2 \), \( \text{O}_2 \), and \( \text{O}_3 \) enables the concentrations of \( \text{SO}_2 \) to reach up to 1 ppm in the stratosphere.

In \( \text{H}_2 \)-dominated atmospheres the high UV environment leads to low abundances of \( \text{SO}_2 \) over the entire atmosphere. We note that strong \( \text{SO}_2 \) abundances in moist, warm tropospheres (see Fig. 2) would favor significant sulfate aerosol formation, although a strong hydrological cycle would quickly wash out the sulfate formed (see, e.g., Loftus et al. 2019).
3.2.8. Potential biosignatures NH$_3$, PH$_3$, CH$_3$Cl, and N$_2$O

The chemical destruction of NH$_3$, PH$_3$, and CH$_3$Cl is controlled by reactions with OH, O$_3$, and H and by photodissociation in the UV (see, e.g., Segura et al. 2005; Seager et al. 2013a; Sousa-Silva et al. 2020). In the middle atmosphere NH$_3$ photodissociates into NH$_2$ and H. In H$_2$-dominated atmospheres the NH$_3$ reacts quickly with H and reforms as NH$_3$. In the high CH$_4$ atmosphere this recombination process is slower due to enhanced HO$_3$ from water photolysis in the stratosphere leading to more destruction of atomic hydrogen by reaction (R5) (see also Sect. 3.2.3). Our results suggest that an assumed emission of 8.38 $\times$ 10$^{10}$ molecules cm$^{-2}$ s$^{-1}$ would lead to NH$_3$ surface mixing ratios between 0.1 and 1 ppm. This is consistent with the results from Seager et al. (2013a), who obtain an NH$_3$ mixing ratio of 0.1 ppm with surface flux of 5.1 $\times$ 10$^{10}$ molecules cm$^{-2}$ s$^{-1}$ for a planet with an H$_2$-dominated atmosphere around an active M dwarf.

For PH$_3$ we assume an emissions flux of 1 $\times$ 10$^{10}$ molecules cm$^{-2}$ s$^{-1}$, and obtain a surface mixing ratio of about 200 ppb for the H$_2$-dominated atmosphere with low CH$_4$ concentrations. Sousa-Silva et al. (2020) find similar mixing ratios of PH$_3$ when assuming a ten times higher surface flux for a planet with an H$_2$-dominated atmosphere around an active M dwarf. However, they did not consider that PH$_3$ may be recycled via chemical reactions with H or H$_2$.

For CO$_2$-dominated atmospheres with low and medium concentrations of CH$_4$ (scenarios 10a, 10b) the destruction of PH$_3$ from H is weaker compared to H$_2$-dominated atmospheres, and we obtain higher surface mixing ratios of several ppm. Given the weak recycling of PH$_3$ from H or H$_2$, our results are consistent with Sousa-Silva et al. (2020) who obtain a mixing ratio of 15 ppm for a ten times higher surface flux. For the high CH$_4$ scenario (10c) our results suggest that high abundances of OH are produced near the surface via

\[ \text{CH}_3 + \text{O}_2 \rightarrow \text{H}_2\text{CO} + \text{OH}, \tag{R28} \]

leading to enhanced destruction of PH$_3$ compared to the other scenarios. The CH$_3$Cl and N$_2$O loss processes are dominated by photolysis in the UV below 240 nm and reaction with O$_3$ (see also, e.g., Grenfell et al. 2013). Due to the low UV environment in CO$_2$-dominated atmospheres, the destruction by photolysis is weaker and the abundances of CH$_3$Cl and N$_2$O are higher compared to the H$_2$-dominated atmospheres.

3.2.9. Atmospheric height

The upper right panel of Fig. 3 shows atmospheric height at the ToA for all simulated scenarios. A central aim of this paper is to investigate whether it is feasible to detect atmospheric molecular features on LHS 1140 b with future telescopes. A large atmospheric height leads to stronger absorption features in transmission spectroscopy and hence to improved detectability of the corresponding species. Due to the low mean molecular weight hence larger scale height of the H$_2$-dominated atmospheres, the ToA at $\sim$0.01 Pa occurs at a height of up to 570 km, whereas the CO$_2$-dominated atmospheres only reach an altitude of about 35 km. The higher stratospheric temperatures for the high CH$_4$ scenarios furthermore lead to an expansion of the atmosphere compared to the scenarios with less CH$_4$.

3.3. Transmission spectra

Figure 4 shows the simulated transmission spectrum of LHS 1140 b for the H$_2$-dominated atmosphere with medium CH$_4$ concentrations (scenario 1b). The contribution from individual molecular absorption bands is color-coded. To detect a spectral band with the JWST, for example, it is important to identify a wavelength range that is not obscured by the absorption of other molecules or haze extinction. The strongest spectral features are due to absorption by CH$_4$. Below $\sim$2 $\mu$m molecular features of H$_2$O and NH$_3$ are obscured by haze extinction, which increases the transit depth to $\sim$90 ppm. Between 2 and 2.5 $\mu$m H$_2$-H$_2$ CIA contributes significantly to the transmission spectrum (see Abel et al. 2011).

Around 3.0 $\mu$m we obtain two absorption features mainly produced by NH$_3$, N$_2$O, and PH$_3$. Absorption by CH$_4$ and H$_2$O is rather weak at these wavelengths. However, between 3.0 and 3.1 $\mu$m C$_2$H$_2$ contributes significantly to the spectral feature (not shown). The absorption by CO$_2$ around 3.0 $\mu$m is significant for atmospheres with mixing ratios of $\sim$1% or more CO$_2$ (not shown). The spectral features of CH$_3$Cl around 3.3 and 7 $\mu$m overlap with absorption by CH$_4$ and H$_2$O. For CO$_2$-poor atmospheres the features from N$_2$O and PH$_3$ dominate the spectrum.
between 4.1 and 4.6 \( \mu m \). However, Earth-like CO\(_2\) levels lead to a strong absorption feature around 4.3 \( \mu m \) (see, e.g., Rauer et al. 2011; Wunderlich et al. 2019).

Between 9 and 12 \( \mu m \) we find strong absorption by PH\(_3\), NH\(_3\), and CH\(_3\)Cl. For H\(_2\)-dominated atmospheres there is a significant contribution from H\(_2\)-H\(_2\) CIA (not shown) to the transmission spectrum (Abel et al. 2011; Fletcher et al. 2018).

In CO\(_2\) atmospheres these features might overlap with absorption by O\(_3\) and CO\(_2\). Many of the simulated atmospheric spectral features of N\(_2\)O, NH\(_3\), PH\(_3\), or CH\(_3\)Cl overlap with other molecular bands, for example CO\(_2\) or CH\(_4\) (see Table 6). However, at some spectral bands these potential biosignatures contribute significantly to the full feature offering the possibility to detect the additional absorption if the abundances of CO\(_2\) and CH\(_4\) are known. Figure 5 shows the simulated transmission spectra of H\(_2\)-dominated atmospheres (scenarios 1a, 1b, and 1c) and CO\(_2\)-dominated atmospheres (scenarios 10a, 10b, and 10c). We take into account the effect of weak extinction from thin hazes (solid line) and from thick Titan-like hazes (dashed line).

For the high CH\(_4\) scenarios the mean transit depth is increased compared to the other two scenarios due to strong absorption by CH\(_4\) and the warm stratospheric temperature which leads to an expansion of the atmosphere. Due to the low molecular weight of the H\(_2\)-dominated atmospheres the spectral features are generally larger than in CO\(_2\)-dominated atmospheres. The extinction by thick haze significantly increases the transit depth at atmospheric windows up to 6 \( \mu m \). Hazes at large altitudes are considered to be the main reason for the

---

### Table 6. Central wavelength, \( \lambda_c \) (\( \mu m \)), of molecular bands from NH\(_3\), PH\(_3\), CH\(_3\)Cl, and N\(_2\)O and spectral features that might overlap or obscure the bands at the corresponding \( \lambda_c \).

<table>
<thead>
<tr>
<th>Species</th>
<th>( \lambda_c ) (( \mu m ))</th>
<th>Overlap</th>
</tr>
</thead>
<tbody>
<tr>
<td>N(_2)O</td>
<td>2.9 ( \mu m )</td>
<td>CO(_2)</td>
</tr>
<tr>
<td>N(_2)O</td>
<td>4.5 ( \mu m )</td>
<td>CO, CO(_2)</td>
</tr>
<tr>
<td>NH(_3)</td>
<td>2.0 ( \mu m )</td>
<td>H(_2)O, H(_2)-H(_2), haze, CO(_2)</td>
</tr>
<tr>
<td>NH(_3)</td>
<td>3.0 ( \mu m )</td>
<td>CO(_2), C(_2)H(_2)</td>
</tr>
<tr>
<td>NH(_3)</td>
<td>6.1 ( \mu m )</td>
<td>CH(_4), H(_2)O</td>
</tr>
<tr>
<td>NH(_3)</td>
<td>10.5 ( \mu m )</td>
<td>H(_2)-H(_2), O(_3), CO(_2)</td>
</tr>
<tr>
<td>PH(_3)</td>
<td>4.3 ( \mu m )</td>
<td>CO(_2)</td>
</tr>
<tr>
<td>PH(_3)</td>
<td>9.5 ( \mu m )</td>
<td>H(_2)-H(_2), O(_3), CO(_2)</td>
</tr>
<tr>
<td>CH(_3)Cl</td>
<td>3.3 ( \mu m )</td>
<td>CH(_4)</td>
</tr>
<tr>
<td>CH(_3)Cl</td>
<td>7.0 ( \mu m )</td>
<td>CH(_4), H(_2)O, C(_2)H(_6)</td>
</tr>
<tr>
<td>CH(_3)Cl</td>
<td>9.8 ( \mu m )</td>
<td>H(_2)-H(_2), O(_3), CO(_2)</td>
</tr>
</tbody>
</table>
observed flat spectrum of GJ 1214 b (Bean et al. 2010; Désert et al. 2011; Kempton et al. 2011; Kreidberg et al. 2014). However, HST observations of the atmosphere of LHS 1140 b suggest a clear atmosphere (Edwards et al. 2021). In the following text we compare the observed spectrum with our simulations.

### 3.4. Comparison to observations

Diamond-Lowe et al. (2020) combined two spectrally resolved transit observations of LHS 1140 b from the optical to the NIR (610–1010 nm). Their median uncertainty of the transit depth is 260 ppm. They concluded that about a factor of 4 higher precision would be needed to detect a clear hydrogen-dominated atmosphere. The strongest spectral feature of CH₄ at ~900 nm has a strength of about 130 ppm assuming weak extinction by hazes (solid orange line in Fig. 5). The slope from extinction by thick hazes between 610 and 1010 nm leads to a decrease in the transit depth of ~50 ppm (dashed orange line in Fig. 5, upper panel). Hence, our results confirm that the precision of transit observations between 610 and 1010 nm shown by Diamond-Lowe et al. (2020) is not large enough to draw a conclusion on the atmosphere of LHS 1140 b.

Recently, Edwards et al. (2021) presented HST transit observations between 1.1 and 1.7 µm. They concluded that a maximum in the spectrum around 1.4 µm might suggest evidence of water vapor absorption in a clear H₂–He atmosphere. However, due to the large stellar contamination and the low overall S/N further observation time is required to confirm the detection of a planetary atmospheric feature. Figure 6 compares the spectrally resolved HST observations with simulated spectra assuming H₂-dominated atmospheres (scenarios 1a, 1b, and 1c). The low CH₄ scenario shows a mixing ratio of H₂O below 1 ppm in the middle atmosphere (see Fig. 2) and the resulting spectrum shows only a weak feature at 1.4 µm (blue line). In Edwards et al. (2021) the water vapor abundance has been retrieved to log₁₀[V(H₂O)] = −2.94±1.45. When assuming an H₂O mixing ratio of 1%, constant over height, we find a difference in the observed transit depth of about 150 ppm between 1.4 and 1.6 µm. However, such large abundances of H₂O are not consistent with the results of our photochemical model simulations for thin H₂-dominated atmospheres with habitable surface temperatures. Large abundances of H₂O in thick H₂-atmospheres, which were not considered here, might be consistent with our model but would lead to surface temperatures above 395 K (see Fig. 1), which are unlikely to sustain life (see, e.g., Bains et al. 2015).

Figure 6 suggests that a large spectral feature of ~200 ppm at 1.4 µm can be also obtained by strong CH₄ absorption in a thin H₂-dominated atmosphere containing several percent of CH₄ and limited haze production. High abundances of CH₄ might favor the formation of hydrocarbon haze (He et al. 2018; Höst et al. 2018; Lavvas et al. 2019). However, Fig. 2 suggests that the haze production is lower compared to CO₂-dominated atmospheres with high CH₄ abundances (see Sect. 3.2.6).

Similarly to our finding regarding the atmosphere of LHS 1140 b, the model studies by Bézard et al. (2020) and Blain et al. (2021) suggest that the detected spectral feature at 1.4 µm in the atmosphere of K2-18 b (Benneke et al. 2019; Tsiaras et al. 2019) might be produced by CH₄ rather than H₂O. They concluded that the H₂O-dominated spectrum interpretation is either due to the omission of CH₄ absorption or to a strong overfitting of the data. Further observations with the Very Large Telescope (VLT) or the JWST are expected to confirm or rule out the existence of large abundances of CH₄ in the atmosphere of LHS 1140 b or K2-18b (see, e.g., Edwards et al. 2021; Blain et al. 2021). In the following we further determine the capabilities of the upcoming generation of telescopes with increased sensitivity and larger wavelength coverage to characterize the atmosphere of LHS 1140 b.

### 3.5. Detectability of spectral features with JWST and ELT

To determine the number of transits that are required to detect a spectral feature (S/N = 5) we subtract the full transmission spectra (including the absorption from all species, CIAs, H₂O CKD, Rayleigh extinction, and extinction from hazes) from the spectrum excluding the contribution from the corresponding species. Thus, we consider only the contribution of these species to the full spectrum. This method assumes that we know the concentration of other main absorbers, such as CH₄ or CO₂, that may overlap with the spectral bands (see Table 6). We note that other molecules could mimic large-scale features of the molecule in question. Hence, retrieval analysis (see Barstow & Heng 2020,
Fig. 7. Simulated transmission spectra of LHS 1140 b with weak extinction from hazes in solid lines as shown in Fig. 5. **Upper panel:** H$_2$-dominated atmospheres with low, medium, and high CH$_4$ concentrations corresponding to scenarios 1a (blue), 1b (green), and 1c (orange), respectively. **Lower panel:** CO$_2$-dominated atmospheres with low, medium, and high CH$_4$ concentrations corresponding to scenarios 10a (blue), 10b (green), and 10c (orange), respectively. The shaded region shows the contribution of the minor species to the full spectrum. Expected error bars for a single transit observation assuming scenario 1c (upper panel) and 30 co-added transits assuming scenario 10c (lower panel) using JWST NIRSpec PRISM (0.7–5 µm) and JWST MIRI LRS (5–12 µm), binned to $R = 30$. Strongest contribution of minor atmospheric molecular absorption bands are indicated by the color of the scenario or in gray when all scenarios have a significant contribution.

for a recent overview) or the detection of the molecules at multiple wavelengths would be required to exclude any ambiguity.

Second, for LRS with JWST NIRSpec we bin the spectral data until the optimal value is found, leading to the lowest required number of transits. On the one hand binning the data decreases the noise contamination, but on the other hand large wavelength ranges can lead to interfering overlaps of absorption bands and atmospheric windows. Due to the unknown systematic error when binning the synthetic spectral data we assume only white noise for the binning. This gives an optimistic estimation on the detection feasibility of the JWST. It should be noted that we do not consider the wavelength range between 1 and 2 µm due to the saturation of the detector for NIRSpec PRISM. However, due to extinction by hazes, the detection of the spectral features of CH$_4$ and CO$_2$ at this wavelength range would require similar or more observation time than the features at longer wavelengths. For the high-resolution spectra we use a constant resolving power of $R = 100,000$, as planned for the HIRES and METIS on ELT, and apply the cross-correlation technique with the same method as presented in Wunderlich et al. (2020). We do not show results from emission spectroscopy in this study due to the much longer required observation time compared to transmission spectroscopy for planets in the habitable zone (see, e.g., Rauer et al. 2011; Lustig-Yaeger et al. 2019).

At most wavelengths the simulated spectra are dominated by major absorbing species (here defined as H$_2$, He, CO$_2$, CH$_4$, and H$_2$O). To identify suitable wavelength ranges for the detection of minor absorbers (here defined as all non-major species), the spectrum including only major absorbers was subtracted from the full spectrum. The remainder, representing the contribution of the minor absorbers to the full spectrum, is shown in the shaded region in Fig. 7. The expected error bars of the simulated H$_2$-dominated atmospheres observed by JWST NIRSpec PRISM or MIRI LRS suggest that a detection of minor absorbers will be challenging within a single transit (upper panel of Fig. 7). However, multiple transits might improve the S/N sufficiently to detect these features.

In CO$_2$-dominated atmospheres the larger molecular weight decreases the features in the transmission spectra compared to H$_2$-dominated atmospheres. The error bars in the lower panel of Fig. 7 arise from 30 co-added transit observations with JWST, which would correspond to a period of two years if each transit of LHS 1140 b were to be observed or ~120 h observing time. The results suggest that it will be very challenging to detect minor absorbers in a CO$_2$-dominated atmosphere during the lifetime of JWST. The detection of major absorbers such as CO$_2$ or CH$_4$ might be feasible, but also challenging. This is consistent with the results of Morley et al. (2017), who suggest that the detection
of a Venus-like atmosphere on LHS 1140 b would require over 60 transits with JWST.

The upper panel of Fig. 8 suggests that CO$_2$ is detectable at 4.3 $\mu$m for mixing ratios between $1 \times 10^{-3}$ and 0.1 within a few transits. For the scenarios 1a, 1b, and 1c with only 1 ppb CO$_2$ the spectral features are too weak to allow the detection of CO$_2$ (see also Fig. 4). The detection of CO$_2$ is only weakly dependent on the amount of CH$_4$ in the atmosphere. The high CH$_4$ cases require fewer transits due to the larger atmospheric heights from CH$_4$ heating in the middle atmosphere (see Fig. 3). The detection of CO will be challenging in the atmospheres we consider. Hydrocarbons such as C$_2$H$_2$ are formed in large abundances for the high CH$_4$ case and could be detectable with fewer than ten transits in CO$_2$-poor, H$_2$-dominated atmospheres.

The number of transits required to detect H$_2$O is smallest for the H$_2$-dominated atmosphere with high CH$_4$ concentration (scenario 1c). This scenario has the lowest surface water vapor, but large amounts of chemically produced H$_2$O in the stratosphere. Hence, the detection of water in transmission spectroscopy is only weakly related to the presence of liquid surface water in these cases.

For each of the atmospheric scenarios we assume a strong dry deposition of CO (see Table 4) leading to weak accumulation of CO from CO$_2$ photolysis in CO$_2$-rich atmospheres compared to previous model studies (Schwieterman et al. 2019; Hu et al. 2020; Wunderlich et al. 2020). Hence, the detection of CO will be challenging in the atmospheres we consider. Hydrocarbons such as C$_2$H$_2$ are formed in large abundances for the high CH$_4$ case and could be detectable with fewer than ten transits in CO$_2$-poor, H$_2$-dominated atmospheres.

For the cross-correlation technique with high-resolution transmission spectroscopy using ELT HIRES or METIS (lower panels). The x-axis of the upper panel is different from the middle and lower panels. Each colored circle corresponds to one scenario from Table 3. Blue lines and circles show low CH$_4$ scenarios, green lines and circles show medium CH$_4$ scenarios, and orange lines and circles show high CH$_4$ scenarios.
medium concentrations of CH$_4$ (scenarios 1a–3a and 1b–3b) the results suggest that the detection of NH$_3$ would require tens to hundreds of transits with JWST NIRSpec PRISM, and the spectral lines of NH$_3$ around 1.5 $\mu$m might be detectable with about five transits with ELT HIRES. The detection of NH$_3$ around 2.3 $\mu$m would require around eight transits (not shown). However, due to the possibility of a simultaneous detection of spectral lines from CH$_4$, H$_2$O, and CO, this wavelength region might be favorable for HRS (Brogi & Line 2019). Strong extinction by hazes or large absorption by CH$_4$ for the high CH$_4$ scenarios would prevent the detection of NH$_3$.

The spectral feature of PH$_3$ at 4.3 $\mu$m might be detectable within 10–30 transits for the H$_2$-dominated atmospheres with 1 ppb CO$_2$ (scenarios 1a, 1b, and 1c) and weak extinction by hazes. For the other scenarios the PH$_3$ feature is obscured by the CO$_2$ absorption band around 4.3 $\mu$m (see also Sousa-Silva et al. 2020). The detectability of PH$_3$ is improved using high-resolution spectra of ELT METIS compared to JWST observations for CO$_2$-rich atmospheres. However, for more than 1% of CO$_2$ mixing ratios the detection of PH$_3$ would require tens to hundreds of transits.

For H$_2$-dominated atmospheres with high concentrations of CH$_4$ (scenario 1c) the mixing ratios of CH$_3$Cl are higher compared to scenarios 1a and 1b (see Fig. 2). However, the strongest spectral band of CH$_3$Cl in the wavelength range of JWST NIRSpec PRISM overlaps with absorption by CH$_4$ (see Fig. 4) owing to a better detectability of CH$_3$Cl in CH$_4$-poor atmospheres. A similar observation time is required to detect CH$_3$Cl with JWST and with ELT for the low CH$_4$ scenarios. However, the cross-correlation technique is less sensitive to the increase in CH$_4$ compared to LRS. We note that ten transit observations with JWST would be feasible within one or two years (given a 24.7-day orbital period of LHS 1140 b, Dittmann et al. 2017), but ground-based facilities would require a much longer observation period because fewer transits could be captured per year. N$_2$O might be detectable within 10 to 20 transits in CO$_2$-poor atmospheres with thin hazes. Results suggest weak dependence of the detectability of N$_2$O on the concentration of CH$_4$.

Our paper suggests that the detection of potential biosignatures with JWST or ELT is feasible for clear, H$_2$-dominated atmospheres, but would require several transit observations. If such a molecule were detected, retrieval analysis might find it challenging to constrain its abundance with low uncertainties, due to sparse knowledge on broadening coefficients (see, e.g., Tennyson & Yurchenko 2015; Hedges & Madhusudhan 2016; Barton et al. 2017; Fortney et al. 2019), and hence it would be difficult to rule out a potential abiotic origin.

4. Summary and conclusion

In this study we used a self-consistent model suite to simulate the atmosphere and spectral appearance of LHS 1140 b. First, we performed climate-only runs to determine the surface pressures for which the super-Earth LHS 1140 b would have habitable surface conditions in N$_2$, H$_2$, and CO$_2$ atmospheres. Our results suggest that a thick N$_2$-dominated atmosphere on LHS-1140 b or substantial amounts of greenhouse gases such as CO$_2$ would be required to reach habitable surface temperatures. A $\sim$2.5 bar CO$_2$ atmosphere or a $\sim$0.6 bar H$_2$–He atmosphere would lead to a surface temperature of $\sim$273 K. In the second step we used these results and assumed a fixed surface pressure of 2.416 bar (corresponding to the atmospheric mass of the Earth) to simulate potential CO$_2$- and H$_2$-dominated atmospheres of LHS 1140 b with our coupled climate-photochemistry model, 1D-TERRA. We simulated the possible composition of the planetary atmospheres, assuming fixed biomass emissions and varying boundary conditions for CH$_4$.

The results suggest that the amount of atmospheric CH$_4$ can have a large impact upon the temperature and composition of H$_2$-dominated atmospheres. A few percent of CH$_4$ may be enough to lower the surface temperatures due to an anti-greenhouse effect. In H$_2$-dominated atmospheres with high concentrations of CH$_4$ this effect dominates, leading to a cooling of up to 100 K, and the stratosphere is pronounced with temperatures up to 70 K warmer than those at the surface. Although we did not consider the effect of hydrocarbon hazes in the climate-chemistry model, Arney et al. (2017), among others, have shown that this is expected to warm the surface temperature by only a few degrees. For CO$_2$ atmospheres the temperature profile is less affected by CH$_4$ absorption due to CO$_2$ cooling in the stratosphere.

In H$_2$-dominated atmospheres O$_2$ is efficiently destroyed preventing significant concentrations of O$_2$ and O$_3$ in such environments. Hence, even if O$_2$ or O$_3$ were biosignatures they would not be detectable in the atmosphere of such a habitable planet dominated by H$_2$. In CO$_2$-dominated atmosphere O$_2$ and O$_3$ can be produced abiotically, which might lead to a false-positive detection (see also Selsis et al. 2002; Segura et al. 2007; Harman et al. 2015; Meadows 2017; Wunderlich et al. 2020). However, results suggest that large amounts of CH$_4$ would also lead to low concentrations of O$_2$ and O$_3$.

We consider NH$_3$, PH$_3$, CH$_3$Cl, and N$_2$O to be potential biosignatures in H$_2$ and CO$_2$ atmospheres. Here the main constituent of the atmosphere has a weak impact on the concentrations of these potential biosignatures assuming that the emission flux is the same for both H$_2$ and CO$_2$ atmospheres (see also Seager et al. 2013a; Sousa-Silva et al. 2020). However, the detectability of molecules with transmission spectroscopy largely depends on the main composition of the atmosphere due to the difference in mean molecular weight.

Observations of the planet suggest that the atmosphere of LHS 1140 b has a low mean molecular weight (Edwards et al. 2021). In a thin, H$_2$-dominated atmosphere our results suggest that the tentative spectral feature at 1.4 $\mu$m might be produced by CH$_4$ rather than H$_2$O. If the feature at 1.4 $\mu$m were produced by water vapor absorption, surface temperatures are unlikely to be habitable. Our results suggest that the molecular features of CH$_4$ and CO$_2$ for habitable surface conditions might be detectable within one transit using JWST NIRSpec observations around 3.4 and 4.3 $\mu$m, respectively. At these wavelengths the absorption cross section of H$_2$O is weak, and at large wavelengths the extinction by hazes has only a weak impact on the detectability of spectral features. The detection of NH$_3$, PH$_3$, CH$_3$Cl, or N$_2$O would require about 10–50 transits ($\sim$40–200 h) with JWST, assuming clear conditions. The molecular bands of these species overlap with absorption by CO$_2$ or CH$_4$ in most cases, making a detection more challenging.

With high-resolution spectroscopy using ELT HIRES or METIS individual absorption lines are distinguishable which might improve the detectability of potential biosignatures. Our results suggest that NH$_3$ might be detectable with less than 20 h of ELT observing time in H$_2$-dominated atmospheres with low or medium CH$_4$ mixing ratios. A thick haze layer in the atmosphere would, however, prevent the detection of any potential biosignature. Strong spectral lines of PH$_3$, CH$_3$Cl, and N$_2$O feature in the wavelength range of ELT METIS with overall lower sensitivity compared to ELT HIRES (see, e.g., Wunderlich et al. 2020). Results suggest that a single transit observation of LHS 1140 b with JWST NIRSpec would be enough to confirm
or rule out the existence of a clear H$_2$-dominated atmosphere, as suggested by recent observations (Edwards et al. 2021). Such an observation would help more accurately constrain the atmospheric CH$_4$. If future observations suggest a thin H$_2$-dominated atmosphere on LHS 1140 b, the planet is one of the best currently known targets to find potential biosignatures such as NH$_3$ or CH$_4$Cl in the atmosphere of an exoplanet in the habitable zone with a reasonable amount of JWST or ELT observation time.

Acknowledgements. This research was supported by DFG projects RA 714/7-1, GO 2610/1-1, SCHR 1125/3-1 and RA 714/9-1. We acknowledge the support of the DFG priority programme SPP 1992 “Exploring the Diversity of Extrasolar Planets (GO 2610/2-1)”. J.L.G. thanks ISSI Team 464 for useful discussion.

We thank Michel Dobrijevic for providing their simulated chemical profiles of Neptune and Titan and discussions on the CH$_4$ atmosphere on LHS 1140 b, the planet is one of the best currently known targets to find potential biosignatures such as NH$_3$ or CH$_4$Cl in the atmosphere with a reasonable amount of JWST or ELT observation time.

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Appendix A: Neptune validation

Neptune validation

The lower boundaries at 100 hPa are set to a constant mole fraction \( f \) for He, CH\(_4\), CO, CO\(_2\), and H\(_2\)O respectively to \( f_{\text{He}} = 0.19 \) (Williams et al. 2004), \( f_{\text{CH}_4} = 9.3 \times 10^{-2} \) (Lellouch et al. 2015), \( f_{\text{CO}} = 1.1 \times 10^{-6} \) (Luszcz-Cook & de Pater 2013), and \( f_{\text{CO}_2} = 5 \times 10^{-10} \) (Feuchtgruber et al. 1993). H\(_2\) is set to be the fill gas in each layer to make up the total volume mixing ratio to unity. For all other species we assume a dry deposition velocity, \( v = K_0/H_0 \), where \( K_0 \) is the eddy diffusion coefficient and \( H_0 \) the atmospheric scale height at the lower boundary. The eddy diffusion coefficient over height \( K_{zz} \) is adapted from Moses et al. (2018):

\[
K_{zz} = \begin{cases} 
10^4 \left( \frac{1}{P} \right)^{0.55}, & \text{if } p \leq 0.5 \text{ Pa} \\
10^2 \left( \frac{1}{P} \right)^{0.98}, & \text{if } 0.5 \text{ Pa} > p > 280 \text{ Pa} \\
400, & \text{if } p \geq 280 \text{ Pa}
\end{cases}
\]  

\[(A.1)\]

Results suggest that the Neptunian atmosphere, as simulated by the photochemistry model, compares well both with the observations and with the results from Dobrijevic et al. (2020) and Moses & Poppe (2017). Observations for pressures below 0.1 hPa, however, suggest a depletion of CH\(_4\), which is not predicted in our model. In the stratosphere of Neptune molecular diffusion is the main process that controls the relative abundance of CH\(_4\) above the methane homopause. The model version applied here includes Eddy diffusion, but not molecular diffusion, consistent with an overestimation of the CH\(_4\) concentrations below 0.1 hPa.

Appendix B: Titan

Titan validation

Figure B.1 shows the composition profiles of selected species in the atmosphere of Titan, calculated with BLACKWOLF and compared to the results from Loison et al. (2019) and Krasnopolsky (2014). The observations are taken from Nixon et al. (2013), Kutepov et al. (2013), and Koskinen et al. (2011).

At the surface (1.45 bar) we set a constant mole fraction \( f \) for CH\(_4\), CO, and H\(_2\), respectively, to \( f_{\text{CH}_4} = 0.015 \) (Niemann et al. 2010), \( f_{\text{CO}} = 4.7 \times 10^{-5} \) (de Kok et al. 2007), and \( f_{\text{H}_2} = 1 \times 10^{-3} \) (Niemann et al. 2010). N\(_2\) is set to be the fill gas in each layer. For all other species we assume a dry deposition velocity of 0.02 cm s\(^{-1}\). The eddy diffusion profile is taken from Krasnopolsky (2014). The temperature profile is taken from Loison et al. (2019).

Our simulated atmosphere of Titan compares reasonably well with the results of Krasnopolsky (2014) and Loison et al. (2019) and is consistent with the observations. We simulate annual and global mean conditions with the model, whereas the measurements do not represent the full range of temporal and spatial variations in the atmosphere of Titan. Profiles of latitudinal variations in the atmospheric composition of Titan are shown in Vinatier et al. (2010), among others.

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\[\text{http://perso.astrophy.u-bordeaux.fr/~mdobrijevic/photochemistry}\]
Appendix C: Representation of thick hazes in GARLIC

We simulate the transmission spectrum of Titan with GARLIC using the output of BLACKWOLF (see Appendix B). Since the ToA for Titan in our model is at ~500 km, we use the data from Loison et al. (2019) to extend the atmosphere up to 1500 km. GARLIC represents the extinction by hazes using Eq. (1). We vary $\alpha$ and $\beta$ to fit the transmission spectrum from Robinson et al. (2014) observed by the Visual and Infrared Mapping Spectrometer (VIMS) from Brown et al. (2004) aboard the Cassini spacecraft. The best fit is presented in Fig. C.1 using $\alpha = 2.6$ and $\beta = 6.0 \times 10^{-25}$. We use these values to simulate the impact of extinction from thick hazes in the atmosphere of LHS 1140 b.

The CH$_4$ absorption features are reproduced well by GARLIC. We underestimate the absorption of the C-H stretching mode of aliphatic hydrocarbon chains near 3.4 $\mu$m (see Bellucci et al. 2009; Maltagliati et al. 2015). This discrepancy is likely due to incomplete line lists or cross sections in the HITRAN 2016 database for several hydrocarbons such as the allyl radical (C$_3$H$_5$; Uy et al. 1998; DeSain & Curl 1999), butane (C$_4$H$_{10}$; Abplanalp et al. 2019) and methylacetylene (CH$_3$CCH; Abplanalp et al. 2019). Furthermore, our chemical network lacks some of the higher hydrocarbons for which absorption cross sections exists, such as isoprene (C$_5$H$_8$; Brauer et al. 2014).

Fig. C.1. Transit transmission spectrum for Titan represented by effective height (in km, blue solid line). The shaded region indicates deviations from four individual transit spectra taken from Robinson et al. (2014). The black dashed line shows the best fit haze model.