Prospects for the characterization of habitable planets

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Guest editors: Anne-Marie Lagrange (LESIA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Sorbonne Paris Cité, 5 place Jules Janssen, 92195 Meudon, France.) and Daniel Rouan (LESIA, Observatoire de Paris, Université PSL, CNRS, Sorbonne Université, Sorbonne Paris Cité, 5 place Jules Janssen, 92195 Meudon, France.)
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Prospects for the characterization of habitable planets

Perspectives pour la caractérisation des planètes habitables

Stephane Mazevet *, a, Antonin Affholder b, Boris Sauterey b, Alex Bixel c, d, Daniel Apai c, d and Regis Ferriére b, e, f

a Observatoire de la Côte d’Azur, Université Côte d’Azur, CNRS, 96 boulevard de l’observatoire, F06304 Nice cedex 4, France

b Institut de Biologie de l’École Normale Supérieure, ENS, Université Paris Sciences et Lettres, Paris, France

c Department of Astronomy, The University of Arizona, Tucson, AZ 85721, USA

d Lunar and Planetary Laboratory, The University of Arizona, Tucson, AZ 85721, USA

e Department of Ecology and Evolutionary Biology, University of Arizona, Tucson, USA

f International Research Laboratory for Interdisciplinary Global Environmental Studies (iGLOBES), CNRS, ENS, Université Paris Sciences et Lettres

E-mails: stephane.mazevet@oca.eu (S. Mazevet), aaffholder@arizona.edu, sauterey@biologie.ens.fr, abixel@arizona.edu, apai@arizona.edu, regis@arizona.edu

Abstract. With thousands of exoplanets now identified, the characterization of habitable planets and the potential identification of inhabited ones is a major challenge for the coming decades. We review the current working definition of habitable planets, the upcoming observational prospects for their characterization and present an innovative approach to assess habitability and inhabitation. This integrated method couples for the first time the atmosphere and the interior modeling with the biological activity based on ecosystem modeling. We review here the first applications of the method to assess the likelihood and impact of methanogenesis for Enceladus, primitive Earth, and primitive Mars. Informed by these applications for solar system situations where habitability and inhabitation is questioned, we show how the method can be used to inform the design of future space observatories by considering habitability and inhabitation of Earth-like exoplanets around sun-like stars.

Résumé. Avec des milliers d’exoplanètes identifiées, la caractérisation des planètes habitables et l’identification potentielle de celles qui seraient habitées est un défi majeur pour les décennies à venir. Nous rappelons en premier lieu la définition des planètes habitables et les perspectives d’observation à venir pour leur caractérisation. Nous présentons ensuite une approche innovante pour évaluer l’habitabilité et l’habitation pour des systèmes extraterrestres. Cette méthode intégrée couple pour la première fois la modélisation de l’atmosphère et de l’intérieur planétaires avec l’activité biologique basée sur la modélisation des écosystèmes. Nous passons en revue ici les premières applications de cette approche pour évaluer la probabilité et l’impact...
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de la méthanogénèse pour Encelade, la Terre primitive et Mars primitive. En se basant sur ces applications pour les situations du système solaire où l’habitabilité et l’habitation sont remises en question, nous montrons comment la méthode peut être utilisée pour éclairer la conception des futurs observatoires spatiaux en considérant l’habitabilité et l’habitation des exoplanètes semblables à la Terre autour d’étoiles semblables au Soleil.

**Keywords.** planets, exoplanets, habitable zone, habitable planets, habitability.

**Mots-clés.** planètes, exoplanètes, zone habitable, planètes habitables, habitabilité.


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A little more than 25 years after the discovery of the first exoplanet [1], we have now identified more than 5,000 objects ranging in size from mercury-like objects to ones that have several times the mass of Jupiter with orbital periods spanning from less than a day to several decades. This broad diversity of planets when considering their size, their composition or their orbital properties largely encompasses what is found in the solar system. Understanding this diversity as well as the nature of the objects detected is currently a major challenge in planetary science. It is generating an intense activity to design new observational strategies for either ground and space observatories as, at present, the majority of planets are detected indirectly, by quantifying their influence on their host stars. Using radial velocities or transit methods [2], the parameters of a given planet are poorly constrained, and are restricted to the mass, the radius and a few orbital parameters. The strongest constraints are obtained when these methods can be combined. Atmospheric characterization, that is the basis of our knowledge of the planets of the solar system, is currently very limited for exoplanets.

Atmospheric characterization of exoplanets has only been obtained in a handful of cases. This corresponds to either giant planets with short periods that can be characterized using transit spectroscopy [3] or, conversely, far-out planets in the giant-brown-dwarf continuum that can be accessed using direct imaging [4, 5]. The upcoming generation of instruments from either ground or space such as, for example, the SPHERE and GRAVITY upgrades [6, 7], the European Extremely Large Telescope (E-ELT), the James Web Space Telescope (JWST) [8] and the upcoming ARIEL mission [9] from ESA, aim at improving this situation by characterizing the atmosphere of smaller objects and at varying distance from their host star. While addressing various questions along the way, such as the atmospheric composition of giant planets, the nature of ocean worlds, of sub-neptunes and super-earths, the ultimate and long term goals of the next generation of instruments is to enable us to quantify the habitability of Earth-like planets and eventually identify inhabited ones. In this paper, we review the current status regarding the prospects for the characterization of habitable exoplanets and present an innovative framework to assess habitability and inhabitation on quantitative grounds so as to inform the design of the next generation of space observatories.
1. Current status on habitable planets

1.1. Definition of the habitable zone

Brought forward by H. Shapley more than seventy years ago [10], the concept of the habitable zone rests on the idea that there exists a region around each star where liquid water can be maintained at the surface of an Earth-like planet. The connection between habitability and liquid water is obviously related to the fact that life as we know it requires liquid water to thrive and develop. This definition of habitability relates to life that resembles what we find on Earth and relates to one of its basic constituents, water. It secondly conveys the idea that life is a surface event that, in turn, may potentially modify the atmospheric composition of the planet if present. Planets with liquid water in the subsurface and protected by an ice layer can also be described as habitable. They may exist outside the habitable zone that is now defined by the possibility of surface liquid water but will not be considered here as they are poor candidates for remote sensing based on atmospheric characterization.

The modern estimation of the boundaries of the habitable zone is obtained by using climate modeling for an atmosphere made of CO$_2$, H$_2$O, and N$_2$ [11]. The inner edge is defined as the distance at which a planet develops a wet stratosphere and loses its water through photodissociation and the escape of hydrogen to space [11, 12]. It is the so-called water-loss limit where the planet enters a wet greenhouse runaway. It occurs before the hard greenhouse runaway limit where the atmosphere absorbs more energy than it can radiate back to space. In this case, the surface temperature rapidly increases beyond one thousand degrees and well above what can be deemed habitable. For today’s solar system, these two limits are estimated to be at 0.97 AU and 0.99 AU using a 1-D climate modeling with a fully saturated troposphere and a cloud free atmosphere [12]. Numerous 3D climate modeling studies have refined these values (see below).

The outer edge of the habitable zone is set by the maximum greenhouse effect that can be obtained by continuously adding CO$_2$ in a H$_2$O-CO$_2$ atmosphere. This can occur when a planet experiences an active carbonate-silicate cycle that can lead to a continuous build-up of CO$_2$. Beyond a certain amount of CO$_2$ in the atmosphere, which reaches around 7-8 bars, CO$_2$ condensates and Rayleigh scattering takes over the greenhouse effect. In this case, the planet experiences cooling instead of warming. 1-D modeling sets the outer limit of the habitable zone at 1.67 AU for today’s sun [12]. Formally, the habitable zone could be extended outward assuming additional greenhouse gases, such as NH$_3$ and CH$_4$, in the atmosphere but most gases will not significantly move the outer limit. The exception is hydrogen that can seriously enhance the greenhouse effect when considering dense atmospheres [13–16].

Similar 1-D climate calculations are used to estimate the boundaries of the habitable zone for other type of stars. These calculations take into account the fact that the luminosity of the star decreases with its mass while its emission spectrum shifts to the red and to larger wavelengths. As the stellar mass decreases, the habitable zone gets closer to the host star and enters a region where the planets are tidally locked (i.e., the planetary rotation and orbit are synchronized). This inner and outer limits obtained using climate calculations set what is called the conservative habitable zone. This estimate has been refined by considering additional greenhouses gases as mentioned above and using complex 3-D climate models such as 3D general circulation models (GCM). The latter take into account various effects such as cloud formation, atmospheric circulation, rotation rate. These 3-D estimates of the habitable zone are within 5 to 7% of the 1-D ones for fast rotating planets like the Earth in the habitable zone of (F, G, K) stars. They predict much larger differences for tidally locked and slowly rotating planets that lay in the habitable zone of (K, M) stars. In this situation, 3-D modeling predicts the inner edge of the habitable zone much closer to their host star.
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Figure 1. Distribution of the currently detected planets with the conservative and optimistic habitable zones as a function of stellar temperature of the host star and the flux received by the planet. The flux received is normalized to the Earth one. This plot is regularly updated and produced by the planetary habitability laboratory at the university of Puerto Rico www.phl.upr.edu.

This estimate of the conservative habitable zone, introduced by Kasting et al. [11], updated by Kopparapu et al. [12, 17] and augmented by 3-D modeling [18] is directly related to the modeling of the long term climate evolution of the inner planets of the solar system [10, 11]. As it might be perceived as too restrictive and prone to modeling shortcomings, it is often associated with another empirical estimate directly tied to observables associated to Venus and Mars. In this case, the optimistic inner edge of habitable zone rests on the observation that the age of Venus young cratering are estimated to be at about 0.7 Gyrs. This provides a lower limit to its water loss by either wet or greenhouse run away. Taking into account the sun luminosity at that time, this sets the boundary for the greenhouse runaway at 0.75AU. On the other side of the habitable zone, the surface of Mars suggests that water may have been present 3.8 Gyrs ago. Considering that the solar luminosity was 75% of its current value, this sets the outer boundary of the optimistic habitable zone at 1.75AU, past the estimate obtained using climate modeling, 1.69AU, suggesting that other greenhouse gases that CO\textsubscript{2} and H\textsubscript{2}O were at play if primitive Mars was habitable [15].

1.2. The nature of the planets identified as potentially habitable

The previous section underlines that the habitable zone is not a planetary property but a region around a given star where planets are at the right distance from their host star to potentially sustain liquid water at their surface provided a given atmospheric composition is present. In this context, potentially habitable planets relates to planets that loosely resemble the Earth, made of iron and silicates and with a water content that can reach up to 50% in mass, and orbiting in the habitable zone of their host star.

This situation is illustrated in Figure 1 that shows a diagram elaborated by the planetary habitability laboratory at the university of Puerto Rico [19]. It displays the distribution of planets...
in the habitable zone (see Section 1.1) detected by the end of 2021 with the habitable zone boundaries discussed in the previous section. The planets are shown as a function of their mass and are categorized following solar system counterparts. The continuum between subterran (Mars), terran (Earth-like), and superterran (Super-Earth-mini-Neptune) are arbitrarily divided in two categories. Terran planets represent objects with radius and mass respectively less than $1.6R_E$ and $3M_E$. Superterran on the other hand are defined with a radius and a mass greater than terran but lesser than respectively $2.5R_E$ and $10M_E$. These two broad categories can be associated to the dip in the size distribution identified in the population of exoplanets detected by the Kepler mission [20]. Analysis of the Kepler data shows a higher occurrence rate of planets at $1.3R_E$ and $2.4R_E$ with a valley at $1.8R_E$ suggesting that there is two distinct populations of planets. Further analysis of the mass-radius relationship of planets currently detected indicates that the first population matches Earth and Venus mean densities while the second population, with lower densities, have a higher fraction of volatiles and up to 50% of water [21]. The latter objects do not exist in the solar system and are sometimes also refereed to as waterworlds [22].

Figure 1 shows that due to observational biases with current detection methods, no Earth-like planets have been detected so far in the conservative habitable zone around F or G type stars. Earth-like planets detected in the conservative habitable zone are around K-stars (3500K<T<5000K) and M-stars (T<3500K). There are 13 objects at present with a highest occurrence around M-stars. This number reaches 20 when considering the optimistic habitable zone. It can be extended to 55 when considering planets with a significant amount of water and categorized as superterran. This estimate of potentially habitable planets shows that so far, about 0.2 % of the planets detected are labeled potentially habitable if we consider Earth-like planets and a conservative definition of the habitable zone. This number increases to 1 % if one considers an optimistic definition of the habitable zone and planets stretching toward mini-neptunes.

The exact number of potentially habitable planets detected can vary depending on the precise criterium used. This is not an issue as it is commonly understood that this definition relates to planets that are potentially habitable and among which only a subset may finally turn out to be truly habitable. It should thus be understood as a way to identify targets for further investigation such as atmospheric characterization. Furthermore, habitability depends on other criteria than the mean density and the flux received from the host star. At first, the stellar luminosity increases during the star lifetime. We saw above that within the habitable zone, a planet will be habitable only if the atmosphere is suitable. For a planet to be habitable and remaining habitable during a significant fraction of time for life to develop requires that the atmospheric composition remains suitable [10, 11].

The build-up and long term evolution of the atmosphere of Earth-like planets is a process that is not fully constrained. It rests on an initial budget of volatiles, primary degassing during the magmatic state and the long term geophysical activity, i.e. the evolution of the interior structure, that involves degassing of various species and possibly various tectonic regimes. The situation is even more uncertain for the planets characterized as habitable at present as they are around M-dwarfs, tidally locked with a formation history and stellar conditions that largely depart from what we know on Earth. Furthermore, when considering habitability from an Earth perspective, it appears relevant to also consider its formation in the context of the history of the solar system [23], the low eccentricity of its orbit, its dynamical stability due to the moon, its rotation rate, interior processes allowing plate tectonics to occur and subsequently its long term carbonate-silicate cycle to name a few particular features. Whether all these particularities are necessary to make a planet habitable is an open question that the atmospheric characterization of exoplanets might help address in the coming decades [24].
1.3. **Upcoming prospects for observational characterization**

The atmospheric characterization of potentially habitable planets has been so far obtained for the TRAPPIST-1 system and for a very narrow IR band (1.1-1.7 µm) using the Hubble Space Telescope [25, 26]. The TRAPPIST-1 system consists of seven planets orbiting a M-dwarf star in a very compact configuration. The densities of these planets are rather comparable and are slightly lower than Earth’s mean density [27]. These planets are clearly terrestrial in nature and three of them are in the habitable zone (d, e, f) [28]. The featureless spectra obtained using the Hubble space telescope could only rule out that the atmosphere of these planets were not made of primordial hydrogen. The limited spectral window available and the sensitivity of the instrument did not allow to identify other volatiles such as H₂O or CO₂. The detection of these elements in the atmosphere of terrestrial planets, which can help validate the concept of habitability, and others, such as O₂ or CH₄ related to biological activity, is just starting.

The challenge ahead can be illustrated by considering the TRAPPIST-1 system in the era of the JWST. The distance of the TRAPPIST-1 system, 12pc, combined with the luminosity of the late M-dwarf star provides a first opportunity to probe the atmosphere of Earth-size terrestrial planets with three of them in the habitable zone. The characteristics of the planetary system suggest that transit spectroscopy could be performed for the seven planets detected so far if the instrument is performing as expected.

A consensus is now emerging that the atmospheric properties could be obtained by using between 10 to 100 transits if these planets have a significant atmosphere [29]. CO₂ can be potentially detected using about 10 transits in a cloud-free atmosphere. This goes up to 20-30 transits if the atmosphere is cloudy. The detection of H₂O is much more challenging if the planets resemble the Earth where the water is concentrated in the troposphere and is in small abundance at the altitude probed by transit spectroscopy. If the atmosphere is different, detection of water vapor is estimated to require at least 60 transits but without giving indication whether liquid water is present at the surface [30–32]. The JWST measurements can potentially give better constraints if the TRAPPIST-1 planets are entering a wet greenhouse runaway by detecting a strong massive oxygen atmosphere resulting from ocean lost. Hence, the prospects of assessing the habitability of TRAPPIST-1 planets using JWST might principally concern the inference of the lack of greenhouse runaway.

If we now turn to biosignatures, O₂, that could constitute a biosignature as it is associated to oxygenic photosynthesis, would require more than 100 transits. Detection of CH₄ could be obtained with 10 transits for TRAPPIST-1e but its connection with biotic activities requires better constraints on the planetary context and to quantify the impact of biogical activity on the planetary conditions to be conclusive [29,33,34]. With the TRAPPIST-1 system accessible 1/3 of the year and the number of possible transits representing a fraction of that time, 65 transits possible for planet b and 5 for planet e, this suggests that the atmospheric characterization of the TRAPPIST-1 system may require a significant fraction of the JWST lifetime. A few other systems presenting a comparable optimum configuration may be identified in the coming years but the identification of exoplanet habitability and potential biosignatures is unlikely with this observatory.

The situation will improve with extremely large telescopes (ELTs) that will start operating toward the end of the decade. ELTs will increase the number of targets accessible around M-dwarfs and maybe K type stars. It may provide a more precise characterization based not only on spectroscopy for transitimg and reflected light measurements but also by using direct imaging. It remains unlikely, however, that observations performed on a single or a few planets will provide compelling evidence of habitability or inhabitation of Earth-like planets [35]. This is due to the difficulties at interpreting a single or even a few observations that necessarily rest on refined
modeling. Following [36] and others, we argue here that definite proof regarding habitability and inhabitation requires a statistical approach to identify trends in population of planets that will enable us to gain compelling evidence for the existence of worlds that are habitable and inhabited. This task might be achieved using the next generation of space observatories based on direct imaging. This corresponds to mission concepts such as the Large UV/Optical/IR Surveyor (LUVOIR) [37] or HABEX [38] that aimed at providing a statistically meaningful sample of objects to probe. The design of the next generation space observatories is underway and there is currently a need to define the requirements these instruments should achieve to test unambiguously habitability and inhabitation of extrasolar planets [39]. To contribute to this question, we consider in next section an innovative approach that addresses the question of habitability, the validation of the habitable zone concept and the question of biosignatures by considering on the same footing the planetary context and the hypothetical biological activity.

2. An integrated approach to assess habitability and inhabitation

Following [35, 36, 39, 40], we support here the idea that the identification of habitability and inhabitation should be achieved by identifying trends in exoplanet populations rather than aiming at a precise characterization of a given planet. Considering the question of biosignatures, we propose that it should be approached by directly coupling the planetary environment with the potential biological activity to account for the viability of potential metabolisms and to include their impact on the atmospheric composition. This contrasts with more conventional approaches that aim at looking at the precise identification of a constituent related to biological activities for a single planet. The case of oxygen that relates to oxygenic photosynthesis illustrates best such an approach [41]. Secondly, we argue that it should be approached statistically as a trend in a population of habitable exoplanets. This formally reduces the possibilities of false positives as it addresses the question of inhabitation of habitable planets as one of their global properties rather than the particularity of a single object.

To bring this approach on a quantitative basis, we developed a model that couples a 1-D photochemical-climate model, an interior model based on a time-dependent parameterization of the carbonate-silicate cycle [42], and an Earth-based ecosystem model to account for the biological activity [34]. This approach expands on the work of Karecha et al. [43] who developed an atmosphere-ecosystem model of the Archean Earth [43]. It also follows on the work of Lehmer et al. [35] who couples a 1-D climate model with a parameterization of the carbonate-silicate cycle to assess trend in population of exoplanets to validate the habitable zone concept. It expands on this work by providing a quantitative modeling of the biological activity that is consistent with the planetary environment. Furthermore, it provides an atmospheric composition that is in turn impacted by the biological activity. To illustrate the features of the approach and demonstrate its usefulness for informing mission designs aiming at identifying habitability and biosignatures for exoplanet populations, we applied it to the case of Enceladus [44], primitive Earth [34] and primitive Mars [45] and to the properties of Earth-like exoplanets around G-type stars [46].

2.1. Enceladus and the Cassini observations

Multiple fly-bys of Enceladus by the Cassini mission confirmed that a global ocean is present [47, 48]. The mass spectrometer onboard the spacecraft also revealed the presence of H₂ and CH₄ among other gases in plumes of gas and ice grains ejected into space at Enceladus’ s south pole. The detection of H₂ was interpreted as a signature of hydrothermal activity [49]. On Earth, alkaline hydrothermal activity produces H₂ and CH₄ among other gases. In Affholder et al. [44], we assume that hydrothermal circulation on Enceladus has its origin in a global ocean harboring
hydrothermal vents and, in turn, that the composition of the plume provides information on the deep-sea vents. Figure 2 (a) shows the interior structure hypothesized for Enceladus with a core heated by tidal dissipation and ocean plumes produced by buoyancy and Coriolis forces [50, 51]. In this configuration, \( \text{H}_2 \) can be produced in Enceladus core by serpentinization [50] while \( \text{CH}_4 \) might originate from the abiotic conversion of \( \text{H}_2 \) and \( \text{CO}_2 \), a primordial stock, or organic molecules present in the core that are pyrolysed.

The biotic origin of \( \text{CH}_4 \) in Enceladus plume has also been largely discussed due to the possible similarities with the Earth's hydrothermal vents [52]. On Earth, these vents host chemosynthetotrophic single-celled organisms - called chemotrophs - that use thermodynamical disequilibrium generated by chemical gradients rather than sunlight as energy sources. Chemotrophic organisms use redox potential as energy source for biomass production. They convert \( \text{H}_2 \) and \( \text{CO}_2 \) into \( \text{CH}_4 \) and could significantly contribute to the production of \( \text{CH}_4 \) detected in Enceladus plume. To test whether these organisms can sustain Enceladus's environment, grow and produce amounts of \( \text{CH}_4 \) compatible with the abundance in the plumes, an ecological model of methanogenesis constrained by the interior environment was developed. The ecological model describes the biomass dynamics of a generic \( \text{H}_2 \)-based methanogenic metabolisms that represent archaea that have been found in Earth's hydrothermal vents. The model is first based on a dependence of the cell metabolism on environmental conditions through the thermodynamics and kinetics of the catabolic (energy-providing) reaction. Catabolic reaction represents the set of reactions a cell uses to maintain itself and grow. The cell population dynamics is described as

\[
\frac{dN}{dt} = N(q_{ana} - d) \quad (1)
\]

\[
\frac{dC_i}{dt} = F(C_i) + NB^* q_{cat} Y_{cat} \quad (2)
\]

where \( N \) is the surface density of the number of individuals in the population (kg\(^{-1}\)m\(^{-2}\)), \( d(\text{s}^{-1}) \) is the baseline death rate, \( B^*(\text{mol}\_c \text{ s}^{-1}) \) is the steady-state internal cell biomass and \( Y_{cat} \) the stoichiometry of the reactants and the products involved. \( q_{ana} \) is the temperature dependent rate of net biomass build-up which sets in turn the division rate. This term depends on the Gibbs free
energy required to produce 1 mol of biomass, the Gibbs free energy dissipated to maintain the cell alive, and $q_{\text{cat}}$ the temperature-dependent rate at which the cell runs the catabolic reaction. $F(C_i)$ is the forcing term setting the concentration of species $i$, $C_i$, given by the modelisation of the planetary environment. In the case of Enceladus, the $\text{H}_2$-based methanogenic population is assumed to be located at the core-ocean interface and $F(C_i)$ represents the concentration calculated in a mixing layer between the hydrothermal fluid and the oceanic water.

This model describes the dynamics of a population of $\text{H}_2$-based methanogens that convert $\text{H}_2$ coming from serpentinization with $\text{CO}_2$ present in the ocean to produce $\text{CH}_4$. The population can reach different steady states depending on temperature and species concentration. This, in turn, sets the efficiency of $\text{H}_2$ consumption and conversion rate into $\text{CH}_4$. It also provides a definition of habitability that corresponds, in this case, to the physical and chemical conditions allowing for a $\text{H}_2$-based methanogen population to grow and reach a steady state. This is defined as the abiotic-habitable conditions. When the population reaches a steady state, it formally modifies the chemical and physical planetary conditions. This is the biotic case that considers the planetary environment inhabited and modified by the population of $\text{H}_2$-based methanogens.

This geochemical and ecological modeling then feeds a statistical hypothesis testing framework by assuming that temperature and the composition of the hydrothermal fluid and ocean (estimated close to 275K) are drawn from prior distributions that encompass uncertainties on their estimates. This includes uncertainties for the serpentinization rate, composition of the ocean for the species of interest and the temperature at the core-boundary. From these prior distributions, input parameters can be drawn for the dynamical model that defines a pseudo-data distribution in the space of observables that corresponds, in the current case, to the flux of $\text{H}_2$ and $\text{CH}_4$ in the plume. Figure 2 shows the distribution of model outputs for the flux of $\text{CH}_4$ obtained by running 50,000 simulations. The model outputs are arranged in the three categories described above, unhabitable, abiotic habitable and biotic depending on whether a methanogen population can grow and reach a steady state. When compared with the Cassini measurements, Figure 2 shows that the observed flux of $\text{CH}_4$ is not reproduced by our abiotic model, but is well within predictions under the assumption of biotic methane production at the seafloor.

This result does not imply that there is an identification of an $\text{H}_2$-based methanogen population at the core-ocean boundary. It indicates that given the abiotic sources of $\text{H}_2$ and $\text{CH}_4$ considered within the planetary model, the fluxes of $\text{CH}_4$ and $\text{H}_2$ observed are compatible with those expected when an $\text{H}_2$-based methanogen population is present given the abiotic situation described. This assumes, first, that the probability of life to emerge for these conditions is significant and, secondly, that no other abiotic process can change significantly the production of $\text{H}_2$ and $\text{CH}_4$ modeled. While these two hypotheses can be challenged, and other can be added, this application illustrates that the framework proposed allows us to do so within the bounds of a quantitative approach where the abiotic and biotic processes are treated on an equal footing and within an integrated approach resting on a direct coupling between the two. We argue that this is a necessary step to identify habitable conditions and design experiments to identify biological activity beyond Earth.

2.2. Primitive Earth and primitive Mars

In Sauterey et al. [34], we apply the approach to quantify the effect of methanogenesis on the atmosphere of primitive Earth. Figure 3 shows that this extends the work for Enceladus described above in several ways. First, the ecosystem consists of not one but several populations of chemotrophic organisms that can develop in the primitive ocean that covers part of the surface of the primitive Earth. Chemotrophs are expected to be the first organisms to develop on Earth, maybe several hundreds millions of years before the apparition of anoxygenic photosynthesis.
Figure 3. (a) Schematic representation of the Earth populated by a basic ecosystem involved in methanogenesis. The parameters that vary during the planet lifetime, $\tau$, are indicated in red. $\Phi_{\text{volc}}(\tau)$ stand for the volcanic outgassing, $\text{Wea}(\tau)$ represents weathering, $P_{\text{CO}_2}(\tau)$ the CO$_2$ surface pressure, $\text{pH}(\tau)$ the ocean pH, and $F_{\text{XUV}}(\tau)$ the stellar flux. (b) Distributions of the CO:CH$_4$ ratio for each plausible evolutionary scenario involving the basic metabolisms considered in the basic ecosystem.

While this hypothesis is still debated, phylogenetic analysis combined with isotopic evidence suggests that this primitive ecosystem may have consisted of H$_2$-based methanogens (MG), CO$_2$-based autotrophic acetogens (AG), and methanogenic acetotrophs (AT). To quantify the effect of methanogenesis on anoxic Earth conditions, we considered these three metabolisms as well as anaerobic oxidation of methane (MT) as a basic ecosystem.

The mean composition and temperature of the ocean and the atmosphere are obtained by using a climate and a photochemical models coupled to a simple temperature dependent carbonate-silicate cycle [42]. The latter computes the evolution of atmospheric CO$_2$, dissolved inorganic carbon (CO$_2$, HCO$_3^-$ and CO$_3^{2-}$) and pH in the ocean by taking into account outgassing from volcanos and mid-oceanic ridges, continental silicate weathering, dissolution of basalt in the seafloor, and oceanic chemistry, as sources and sinks of CO$_2$. This coupled ecosystem-thermal model is solved by considering that the atmospheric temperature and composition and vertical structure reach equilibrium instantly compared to the biological and geological timescales. Secondly, it considers that the dynamics of the ecosystem that occurs in days to years is much faster than the geological time scale ($10^3$-10$^6$ yrs). As previously, the ecosystem dynamics is obtained by considering fixed environmental conditions but given, in this case, by a forcing term, $F(C_j)$, that results from ocean circulation and atmosphere-ocean exchanges and calculated using a stagnant boundary layer model [43]. The steady-state is obtained by considering the biogenic fluxes between the surface ocean, the atmosphere, and the deep ocean iteratively within the planetary model. Once the global steady-state is obtained it represents the coupling between the biotic activity that modifies the planetary conditions that, in turn, feeds back into the efficiency of the biotic activity.

Applied to the case of primitive Earth, we first found that chemotrophic activity had a significant impact on the surface conditions of the anoxic Earth well before nonoxygenic photosynthesis appeared and despite a rather small biomass production. The impact is the strongest on short time scale, 100Myrs, when a new metabolism is introduced or removed from the atmosphere. This can lead to transient warming or ice ball events. On longer time scales, the carbonate-silicate cycle that includes the effect of the biological activity through its dependence on temperature keeps the surface conditions habitable with temperature close to what is expected without
biological activity but with a different state for the atmospheric composition. The imprint of the individual metabolism on the atmospheric composition and surface temperature is clear but converges to a common state when the ecosystem becomes more complex and several metabolisms are included. Figure 3(b) illustrates this situation when considering the CO/CH$_4$ ratio of these two species in the atmosphere. We see that the atmospheric composition changes as soon as a metabolism is included but the footprint of the individual metabolism washes out when the ecosystem becomes more complex to leave a clear signature between abiotic and biotic biospheres.

This study shows that the atmosphere of the anoxic Earth was modified as soon as life emerged. The direct coupling between the ecosystem dynamics and the planetary conditions further allowed us to quantify how methanogenesis impacted planetary conditions, showing that Earth remained habitable on geological time scale. A similar model applied to the case of primitive Mars showed that methanogenesis likely drove Mars out of habitability if these primitive metabolisms appeared [45]. This quantitative modeling suggests a very different outcome between the Earth and Mars upon the potential apparition of methanogenesis, stressing the need for an integrated approach to address habitability and inhabitation on the same footing. This also shows that habitability is, to some extent, determined by inhabitation. The common steady state obtained for primitive Earth in the biotic case, distinct from the abiotic one, and reached as the ecosystem becomes more complex, suggests that a biosignature can be defined. As shown in Figure 3(b), this biosignature is rather independent of the particular characteristic of the metabolisms involved suggesting that this could be used as a biosignature of methane cycling biospheres for future surveys of habitable planets.

2.3. Earth-like population around G-type stars

We now consider the case of Earth-like planets around G-type stars to illustrate how an integrated ecosystem-planetary model can be used to inform the design of future space telescopes aiming at characterizing habitability and inhabitation of extrasolar planets. We saw in the first section that the definition of the conservative habitable zone rests on climate modeling that embodies the greenhouse effects of H$_2$O and CO$_2$ present in the atmosphere. While not explicitly included, it assumes that a carbonate-silicate cycle that regulates the amount of atmospheric CO$_2$ needed to keep the planet habitable exists as the stellar luminosity increases during the host star lifetime [10, 11]. By demonstrating that a population of Earth-like planets follows the general concentration of CO$_2$ anticipated would first validate the concept of habitable zone. It would secondly indicate that these planets may have liquid water on their surface as the carbonate-silicate cycle as we experience it on Earth depends on having liquid water at the surface. Incidentally, it would also confirm how the Earth stayed habitable for 4 billions years (4Gyrs). This approach was suggested by Lehmer [35] and implemented in a very simplified way to validate the habitable zone concept.

The integrated ecosystem-planetary model we developed for the case of primitive Earth allows us to go a step further by not only considering the evolution of the CO$_2$ concentration as a function of time but by also following the complete evolution of the biosphere coupled to the carbonate-silicate cycle. The results shown in the previous section indicate that this may be necessary as habitability and inhabitation are strongly coupled with inhabitation modifying habitability. This approach also provides an appealing way to identify inhabited planets as biosignatures, such as the CO/CH$_4$ ratio mentioned above, can be used and interpreted by fully accounting for the planetary context.

Figure 4 shows preliminary results considering a primitive ecosystem consisting of a single and the same generic methanogen as the one used for the case of Enceladus. Each point shown
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Figure 4. Results of simulated steady state atmospheres displayed as a function of the CO$_2$ surface pressure, $P_{CO_2}$, CH$_4$ surface pressure $P_{CH_4}$, surface temperature, $T$, and time, $t$. The red and blue lines indicate Earth-like planets with densities respectively close to the Earth ($0.9 < \rho < 1.1$) and defined as terran (see Section 1.1) anticipated as detectable using an instrument configuration corresponding to LUVOIR-A.

In Figure 4 corresponds to a complete simulation involving a similar calculation as performed for the case of primitive Earth, coupling photochemistry, climate, the carbonate-silicate cycle and ecosystem modelings and taking into account the variation of volcanic outgassing, weathering and solar luminosity over 4.5 Gyrs as indicated in Figure 3. We note that several technical adjustments are needed to achieve this generalization of the primitive Earth model discussed above over 4.5 Gyrs [46]. Most of them remove simplifying assumptions for the atmosphere-ocean-ecosystem model that are no longer valid when considering the large parameter space explored over such a long time scale, $\tau$.

In Figure 4, the simulations are displayed in three categories. The simulations leading to a surface temperature above 273K are tagged as habitable-temperate as surface temperature is the only criteria used. Following what was done for Enceladus, simulations where a methanogen population can reach a steady state are tagged as habitable for the methanogen population. This represents a fraction of the habitable-temperate set as in addition to temperature, the ocean composition enters in defining the viable conditions for methanogens. Finally, the third set of simulations, habitable-biotic, represents the conditions where the ecosystem activity feeds back into the atmospheric composition. It represents the steady state reached by the ecosystem-planetary system at a given time, $\tau$, given by the stellar luminosity, volcanic outgassing and weathering. The latter two are obtained by the parameterization of the Earth carbonate-silicate cycle [42] while the variation of stellar luminosity and spectrum follow the parameterization of Claire et al. [53]. We note that each simulation point is calculated independently.

Figure 4 shows the variation of the surface temperature and of the CO$_2$ and CH$_4$ surface pressures as a function of time and corresponding to the three sets defined above. We see in
Figure 4 (c) that the amount of CO$_2$ decreases as time evolves and the stellar luminosity increases to maintain habitable conditions. We note that the Sun luminosity increases by 25% over 4 Gyr in these simulation sets. This trend in the atmospheric concentration of CO$_2$ as a function of time represents the effect of the carbonate-silicate cycle. This variation also translates into a varying concentration of CO$_2$ across the habitable zone. Figure 4 (e) shows that the methanogenic population brings an almost constant increase of CH$_4$ in the atmosphere. This biogenic activity is associated to an increase in surface temperature that can be seen in Figures 4 (d)-(f) due to the greenhouse effect of CH$_4$. Inspection of Figure 4 indicates that clear trends exist for the evolution of the atmospheric concentration of CO$_2$ and CH$_4$ over time that may allow us to identify habitability and inhabitation in population of exoplanets. We note that habitability and inhabitation can be accessed independently by considering respectively the habitable temperate and habitable-biotic sets.

If we take the history of life on Earth and its impact on the atmospheric composition of the planet as a template, biogenic CH$_4$ due to chemotrophic activity and non-oxygenic photosynthesis was dominant for more than 1 Gyr. It was followed by a rise in oxygen related to the apparition of oxygenic photosynthesis in two steps, with detectable amount in the atmosphere only 800 Myrs ago. The trends identified in this preliminary calculation correspond to planets that exhibit a carbonate-silicate cycle similar to the one experienced by the Earth and a methanogenic population pertaining over 4 Gyr without the emergence of non-oxygenic and oxygenic photosynthesis. These preliminary simulations can be expanded to explore more thoroughly the parameter space when chemotrophic metabolisms are at play. Photosynthetic metabolisms could be formally included in the approach but require substantial modifications of the ecosystem formalism. The simulations show nevertheless that priors can be built to be used in a Bayesian analysis scheme using a population of potentially habitable planets.

Figures 4 (c)-(e)-(f) illustrate this approach by displaying the exoplanet yield for Earth-like planets around G-type stars expected from the next generation of space telescopes. The sets of exoplanets shown are obtained by using the Bioverse scheme [39, 40] and considering a configuration similar to the LUVOIR-A mission concept [37]. The Bioverse scheme simulates planetary systems for host stars in the solar neighborhood based on the Kepler statistics [54, 55]. The first set displayed in Figure 4 corresponds to planets anticipated in the habitable zone, with densities between 0.9 and 1.1 the Earth one, and potentially detectable using direct imaging. This set corresponds to planets very close to the Earth and could be associated to Earth twins. At first glance, these planets would have a higher probability of displaying a carbonate-silicate cycle similar to the Earth. The second set considers a less restrictive definition and corresponding to the one given in Section 1.2 to define terran planets. We see in Figure 4 that considering planets with densities very close to the Earth, the detection of only eight planets are anticipated with this particular telescope configuration. This number significantly increases when considering planets with a less restrictive density criteria. These precise numbers may be refined in the near future as more surveys come along but it gives a good estimate of the number of candidates that can be expected. Considering that the space observatory has the ability to detect these levels of atmospheric CO$_2$ and CH$_4$, Figure 4 shows that the number of planets anticipated with a configuration corresponding to LUVOIR-A will likely be too low to identify a trend in the variation of CO$_2$ as a function of time for planets with densities very close to the Earth one. The configuration of the LUVOIR-A mission concept may, in contrast, be sufficient to identify methanogenesis if all the candidates display a constant and similar level of CH$_4$ or by considering planets defined as terran with physical properties departing from Earth twins.

This example illustrates how these studies can be used to design instruments and devise observational strategies aiming at identifying trends in populations of exoplanets. For example, the carbonate-silicate cycle as parameterized for the Earth depends on the ability of a planet to
maintain liquid water at its surface. Detecting trend in CO$_2$ as displayed in figure 4 instead of wa-
ter in the atmosphere are two different approaches that could formally be used to identify hab-
itable planets. This leads to two different designs for the space observatory. Furthermore, when
considering the atmospheric concentration of CO$_2$ of a population of planets in the habitable
zone of G-type star and with densities close to the Earth, we see that the statistical set expected
is too limited when considering the configuration of the LUVOIR-A mission concept. This can
be overcome by considering a radically different approach for the design of the space observ-
atory [56]. Conversely, the planet sample can be expanded by considering a less restrictive defi-
nition of Earth-like planets to include a larger variation in mass, radius and density as displayed
in Figure 4. This, however, requires that the current modelisation folds in the dependance of the
carbonate-silicate cycle on these parameters to identify trends. Alternatively, it can also be ap-
proached by using a larger set of stars involving different types and considering luminosity in-
stead of time. Considering planets with a carbonate-silicate cycle driven by different geophysical
regimes such as plaque tectonics like on Earth or a stagnant lid regime like on Venus may also
device a better observational strategy than considering a log-linear relationship between lumi-
nosity and CO$_2$ concentration as suggested in [35]. Overall, we see that the ecosystem-planetary
model developed used in combination with the Bioverse simulations provides a powerful tool to
address these questions quantitatively and progress toward the identification of habitable and
inhabited planets.

3. Summary

The characterization of habitable planets and the possible detection of biotic activity is a major
challenge for the coming decades. It will likely require the development of a new generation
of space telescope optimized to identify trends in population of exoplanets rather than focused
on the precise characterization of a few objects. The design as well as the future analysis of
these experiments require a new generation of models that integrate the coupling between
the potential biotic activity, the atmospheric and interior evolution of terrestrial planets that
expand beyond the Earth size and density. We develop such an approach that couples an
Earth-based ecosystem and planetary modeling. We demonstrated that is is applicable to
identify biotic activity and quantify its effect on habitability for Enceladus, primitive Earth and
primitive Mars, as well as for a population of Earth-like planets around G-type stars. The
latter represents a preliminary analysis that can be expanded in several directions to asses
trends in population of exoplanets that can potentially bring the concept of habitable planets
to observational confirmation.

Conflicts of interest

The authors have no conflict of interest to declare.

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References
