ASTROCHEMISTRY

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The Virtual Planetary Laboratory: Towards Characterization of Extrasolar Terrestrial Planets

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Abstract. NASA and ESA are currently undertaking mission studies for space-based observatories designed to search for life on other worlds. To optimize the designs of these missions, and to ultimately interpret the data sent back by them, we need to recognize habitable worlds and to discriminate between planets with and without life based only on remotely-sensed information. This paper provides an overview of the characteristics we would look for on an extrasolar terrestrial planet that might indicate habitability or the presence of life. It also describes a new NASA Astrobiology Institute research project to develop an innovative suite of modeling tools to simulate the environments and spectra of extrasolar planets. These modeling tools will constitute a Virtual Planetary Laboratory, which will be used to explore the plausible range of atmospheric compositions and globally-averaged spectra for early Earth and for plausible terrestrial planets both with and without life. Products of this research will provide an improved basis for recommending spacecraft and instrument characteristics, as well as search strategies required to remotely sense the signs of life in the atmosphere or on the surface of another world.

1. Introduction

Motivated by the discoveries of over a hundred extrasolar jovian planets, NASA and ESA have initiated a series of mission concept studies for space-based observatories that will search for and characterize life on extrasolar terrestrial planets. These missions will address one of astrobiology's fundamental questions, "Are we alone?". They will also provide an improved census of habitable planets in the vicinity of Earth. To optimize the designs and search strategies for these missions, and to ultimately interpret the remote sensing observations that they return, we must have the capability to recognize worlds that might have habitable conditions, and to discriminate between planets with and without life.

The nascent field of extrasolar planet characterization is necessarily theory-based, given that existing observing techniques are not yet sensitive enough to directly detect and gather information on Earth-sized planets around other stars. This new field seeks to improve our understanding of the potential range of characteristics for terrestrial planets in our galaxy, and the spectroscopic signatures

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that we are likely to encounter. Many of the remote sensing techniques that have been developed to study the Earth and other planets in our solar system could be adapted for use in the characterization of terrestrial planets around other stars. Some of these techniques include *(i)* time-resolved whole-disk photometry, *(ii)* spectroscopic remote sensing for the detection and retrieval of atmospheric and surface composition and physical parameters, and *(iii)* time-resolved spectroscopy of spectral features to look for diurnal or seasonal variations in surface albedo or atmospheric composition.

2. Characterization of Extrasolar Terrestrial Planets

2.1. The Planetary System Environment

When an extrasolar terrestrial planet is first detected via direct astronomical observation, its initial characterization will involve those aspects of its planetary system environment that may affect its potential for habitability. These include, but are not limited to: the spectral type and luminosity of its parent star, the planet's orbital characteristics and its placement in the solar system relative to the star, the type and relative position of other planets in the system, and whether or not the candidate planet has rings or moons, if this can be determined.

2.2. Photometry and photometric variability

Once the solar system environment is understood, additional information about an extrasolar planet can be extracted via its photometry and photometric variability. Time-resolved, disk-averaged photometric observations have provided a wealth of information about planets in our solar system. An understanding of the information content of the characteristic lightcurves derived from these observations is important for understanding what might be learned from photometric observations of extrasolar planets. The planet's apparent brightness and its variability over time in one or more wavelength ranges can be used to determine its effective temperature, and its "color" could provide clues to the composition of its surface and atmosphere. Time-resolved photometric observations acquired as the planet rotates may reveal variability in brightness or color that could indicate the presence of clouds or surface variations. Photometric observations acquired as the planet moves along its orbit track may also provide a way to discriminate between diurnal and seasonal variations. Studies of the potential photometric variability due to rotation of an Earth-like planet at visible wavelengths have been undertaken by Ford et al. (2001).

2.3. Remote Sensing Spectroscopy

Although photometric measurements could yield valuable information about an extrasolar terrestrial planet, by far the most powerful technique available for retrieving the characteristics of planetary surfaces and atmospheres is spectroscopy. As ultraviolet (UV), visible, and near infrared (NIR) radiation from the parent star is scattered and reflected from the planet, the constituents that make up its surface and atmosphere contribute spectral distinct spectral features that provide clues to their composition and physical properties. The radiation

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emitted in the infrared (IR) and microwave regions provides additional spectral information that can be used to characterize the planet's surface and atmosphere. Spectra of the Earth and other planets, acquired over a wide range of wavelengths, have yielded a great deal of information about the structure and composition of the atmosphere and the properties of the underlying surface. However, the first generation instruments for studying extrasolar planets are expected to provide only disk-averaged spectra with modest spectral resolution and signal to noise. We therefore need to understand the information available from disk-averaged spectra of terrestrial planets. Specific examples are provided in the following sub-sections.

Bulk and Trace Atmospheric Constituents Remote-sensing techniques can be use to detect a planetary atmosphere, and determine its bulk and trace constituent composition. Ironically, Earth's principal atmospheric constituent, N_2 has no strong spectral signature throughout most of the spectrum, except in the far UV, and is undetectable by direct methods. However, most other constituents of terrestrial atmospheres, such as H_2O CO_2, O_3, N_2O, NO_2, NO, CO, CH_4, O_2, etc., do produce distinctive spectral signatures at UV, visible, or infrared wavelengths (Fig. 1). If the infrared vibration-rotation bands of these gases can be observed at sufficiently high spectral resolution, the presence of a bulk component that is a radiatively inactive gas (like N_2 in the Earth's atmosphere) can be inferred if it contributes significantly to the pressure broadening of the absorbing species.

Atmospheric Mass The atmospheric pressure at the emitting level in an atmosphere can be retrieved from moderate resolution spectra (1 to 2 cm^{-1}) by modeling the effects of pressure broadening on infrared vibration-rotation bands of absorbing gases. If the planet's atmosphere is sufficiently transparent that radiation can escape from the surface, (e.g., Earth or Mars), the total mass of the atmosphere can be derived. For opaque atmospheres, (e.g., Venus or the Jovian planets), this measurement will yield constraints on the total atmospheric mass above a cloud deck or other opaque surface. In many such cases, observations at UV, visible, and IR wavelengths will indicate different effective pressures, providing additional constraints vertical structure of the atmosphere. This information is important both for studies of the planet's climate (i.e., whether or not it lies within the habitable zone) and for quantifying the trace gas mixing ratios for studies of the atmospheric chemistry (i.e., whether the atmosphere is in chemical equilibrium).

Atmospheric Temperature Once the bulk constituents and "surface" pressure of an atmosphere have been estimated, the thermal structure of the atmosphere can be derived from thermal emission spectra. Comprehensive, spatially resolved temperature measurements would be needed for detailed investigations of the planet's atmospheric dynamics, but even global scale constraints on the atmospheric thermal structure would be valuable for studies of the planet's climate and chemical equilibrium. For example, estimates of the globally-averaged surface temperature would be useful for determining directly whether liquid water is stable on the surface. A broad range of temperature retrieval algorithms have be developed for routine use in cloud-free conditions on Earth (Chahine 1968;

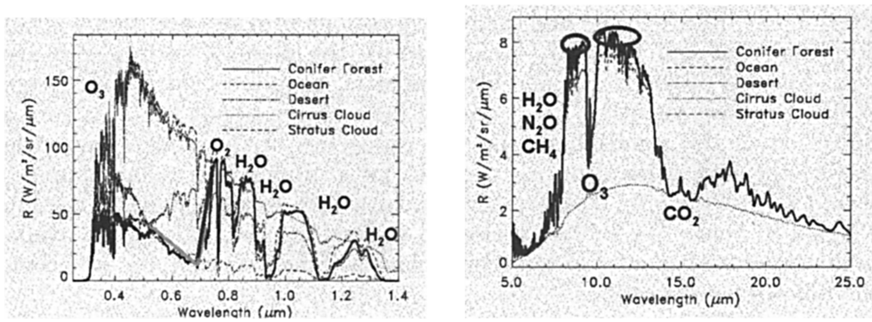

Figure 1. The Earth's Biosignatures. Synthetic spectra of clear and cloudy terrestrial environments at solar (left) and thermal (right) wavelengths generated with the VPL's spectral mapping atmospheric radiative transfer (SMART) model. a) Synthetic solar reflection spectra of clear atmospheres over a conifer forest (solid line), a clear atmosphere over ocean (short dash line), clear sky over desert (dash-dot line), and for a sounding that includes a moderately thick (optical depth = 10) cirrus ice cloud over an ocean surface (dotted line). In each case, the sun is 60^o from the zenith. Chlorophyll, a potentially important biosignature, has strong absorption in the UV and blue (¡0.5μm) and in the red (0.6-0.7μm - marked), and slightly less absorption in the green (0.55μm). Due to changes in the refractive index between air and the internal leaf structure, plants are also highly reflective just beyond the visible range (¿0.7 μm), resulting in a discontinuity (marked) known as "the red edge" (e.g., Elachi 1987; Short 1982). Ozone (¡0.3 μm), water vapor, and the O_2 A-Band at 0.67μm are also prominent in the Earth's solar spectrum. However, high clouds can hide most of these features. B) Synthetic thermal spectra of the environments described above. At these wavelengths, the spectrum is dominated by water vapor, ozone and CO_2 absorption, but is much less affected by surface cover. Reduced gases, such as CH_4 also absorb at these wavelengths, but their spectral signatures are far more subtle than their spectral features at solar wavelengths.

Rodgers 1976), Mars (Conrath 1972; Santee & Crisp 1993), and for the Jovian planets (Conrath et al. 1998). More advanced methods, for use in strongly scattering atmospheres (e.g., Venus and Mars) are also under development. Methods specifically adapted for the analysis of full-disk spectra of heterogeneous objects such as the Earth are also needed.

Phase and Seasonal Variations in Spectral Features In a similar manner to the photometry, time-resolved spectroscopic observations may reveal variations in surface and atmospheric composition that are linked to diurnal or seasonal variations, and may also be produced by the presence of life. For example, time-resolved spectroscopic observations of the Earth would reveal temporal variations in the atmospheric CO_2 and CH_4 abundance that are correlated with seasonal variations in the respiration and photosynthesis of land plants.

Temporally-resolved spectroscopic measurements will also be of particular value for revealing spatial information in disk- averaged observations. Such measurements could provide constraints on the spatial diversity of major continents and oceans. Variations in the retrieved atmospheric temperature or pressure variations could also yield information about global scale weather systems, or seasonal variations in the total atmospheric mass, like those that characterized the Martian atmosphere.

2.4. Astronomical Biosignatures

In addition to characterizing the planet for potential habitability, it is of extreme interest to also look for signs that the planet is inhabited. These signs of life that can be inferred from remote-sensing or astronomical measurements are called "astronomical", or "remote-sensing biosignatures". These could take the form of photometric or spectral signatures that are seen in a certain combination, or exhibit temporal behavior that is considered indicative of life.

Some of the most overt astronomical biosignatures on our own planet are spectral features indicating the presence of surface plants, and the abundant oxygen in the atmosphere. However, many of these astronomical biosignatures have only been characteristics of the Earth's spectrum for about half the time that the Earth has supported life. The Earth's spectrum and any astronomical biosignatures detectable before the advent of oxygen-producing life are currently not well-understood. The simultaneous presence of strongly oxidized and reduced gases that are not in chemical equilibrium (e.g. O_2 and CH_4 in the Earth's atmosphere, Lovelock & Margulis, 1974) is thought to be a robust biosignature for many different kinds of planetary atmospheres. However, these robust indicators are generally much harder to detect via astronomical (remote-sensing) techniques.

2.5. Wavelength Considerations: Optical and Near Infrared vs the Mid Infrared

Initial work on the detectability of astronomical biosignatures focused principally on a narrow range in the mid-infrared. This was driven by initial designs for missions like Terrestrial Planet Finder, which were constrained by astronomical and technical implementation considerations to favor observations in the mid- infrared. At these wavelengths, the contrast between the radiation from the planet and its parent star is down by a factor of 1000 compared with the contrast in the optical, thereby providing higher signal to noise (S/N) information about the planet (Beichman et al 1999). However, new studies indicate that coronagraphic techniques operating in the visible and near-IR can also provide the required S/N, and provide a means to search for biosignatures over a promising spectral range for which there are currently few focused studies on their detectability (see DesMarais et al. (2001) for a study of MIR and optical signatures). There are also several very good scientific reasons for considering spectral ranges other than those in the mid-IR, which are described below. Figure 1 shows a comparison of synthetic spectra generated for the Earth's atmosphere at mid-infrared and optical/NIR wavelengths.

Detection of Disequilibrium Biosignature Pairs The mid-IR region is not optimal for detection of classic disequilibrium biosignatures (like CH_4S or N_2O in the presence of O_2). These disequilibrium biosignature features are much more obvious at optical and near-infrared wavelengths, as already demonstrated during the Galileo flyby of Earth (Sagan et al 1993), and are more robust indicators of life, than a detection of O_3 alone. These classic biosignatures are difficult to detect at mid-IR wavelengths for 2 reasons: 1) O_2 has no prominent spectral features in the mid-IR. At these wavelengths, the presence and concentration of O_2 must be inferred from detection of O_3, which models indicate rises to appreciable concentrations even at relatively low O_2 levels (Kasting & Donahue 1980). Inferring O_2 abundance from O_3 may or may not be robust in atmospheres with different chemical composition and incoming solar flux to our own 2) CH_4 is difficult to detect in the presence of water vapor without high signal to noise (S/N 100) and spectral resolutions much higher than 1000 because in the mid-IR the absorption features are strongly overlapped.

Detection of Surface Composition and Biosignatures Another reason to seriously consider the optical wavelength regime in addition to the mid-IR is that although the mid-IR region is sensitive to both surface temperature differences and trace gas abundances, it is extremely insensitive to underlying surface composition. This is due in part to the relatively small "atmospheric windows" to the surface in the MIR range (see Fig. 1), but is principally due to the lack of spectral features and the uniformly high emissivity of virtually all surface types (ocean/land/vegetation) at these wavelengths. (In analysis of mid-IR remote-sensing data of the Earth, the emissivity of virtually all surfaces is routinely set to 1.0 as an acceptable approximation). However, as shown in Fig. 1 the optical and near-infrared regions of the spectrum display a rich array of spectral features associated with surface composition. With optical observations taken at a set of discrete wavelengths, we could detect chlorophyll on the surface and distinguish between a world dominated by oceans, desert, or forest.

Sensitivity to Cloud Cover Another factor that must be considered when defining the optimum wavelength region for observing biosignatures is the potential loss of information due to persistent cloud cover. Clouds can be associated with convection and condensation of a volatile species, like the water ice clouds seen in the atmosphere of the Earth or the CO_2 clouds seen on Mars, or they can result from photochemical processes, like the planetwide haze layers , which dominate the atmospheres of Venus and Titan. As we show in Fig. 1, high altitude cirrus clouds high in the Earth's atmosphere can obliterate even a strong signal due to O_3 at thermal wavelengths, although clouds at lower levels still allow the detection of O_3. On the other hand, in the visible, the strong A-band of O_2 is always visible in oxygen rich atmospheres, even in the presence of high cloud, although its contrast is somewhat reduced.

Although the photochemical hazes that shroud Venus and Titan are opaque at visible wavelengths, they display "atmospheric windows" at near-IR wavelengths (Meadows & Crisp 1996; Smith et al. 1996) which allow penetration and remote-sensing of the underlying planetary surface. For Venus, thermal radiation from hot surface and lower atmosphere escapes through the clouds and can be detected on the night side of the planet. In the case of Titan, the haze is sufficiently transparent at near-IR wavelengths the surface can be detected even when the satellite is fully illuminated.

Although the mid-IR and the optical/Near-IR have many different characteristics, neither region yet shows a clear advantage for detection of biosignatures or planetary characteristics. In fact, it would be highly desirable to characterize planets in more than one wavelength range, to reduce spectral confusion due to overlapping spectral features associated with different constituents in the system.

2.6. Simulating Planets and their Spectra

To better understand the range of plausible terrestrial planet environments and characteristics that we might encounter in future observations, a theoretical field is under development, which seeks to understand and model the appearance of a broad range of terrestrial planets as seen from space.

The spectrum of a planet is the product of the complex interplay of a range of environmental components and processes. Hence, to generate realistic spectra of a range of plausible extrasolar terrestrial planets we must simulate planetary environments that include these factors. The models used to generate these conditions must be consistent with known physical, chemical, and biological processes. The basic components include: incident solar/stellar flux, thermal structure and composition of the atmosphere including gases, clouds and aerosols, surface properties (land/ocean/ice/biology. In addition, the evolution and equilibrium state of a planet's environment are governed by a series of coupled physical, chemical, and biological processes. These processes include atmospheric and surface radiative heating and cooling rates, atmospheric thermal and photochemistry, impacts and atmospheric escape, the hydrological cycle (oceans, clouds), geological processes such as volcanism, tectonics, weathering and life processes such as respiration and photosynthesis

2.7. The Virtual Planetary Laboratory

To better understand the plausible range of extrasolar terrestrial planets, and their appearance to astronomical instruments, we are currently developing the Virtual Planetary Laboratory (VPL). The VPL is a suite of computer models that will allow our 28 member team to incorporate all of the components and processes outlined above, to simulate a broad range of planetary environments both with and without life, and to determine the spectral signature of these environments. The interrelationship of the various VPL computer models is shown in Fig. 2, and a detailed description of the VPL concept can be found in Meadows et al. (2001).

The core of the VPL is a coupled radiative transfer/climate/chemistry model, which is being assembled using existing models that have been validated individually to address key scientific problems in planetary and Earth sciences. This coupled-climate-chemistry model will be augmented by interchangeable modules, which are also currently under development. These modules will characterize fluxes at the upper and lower boundaries of a planetary atmosphere, and so will consist of geological, exogenic, atmospheric escape, and life processes. The integrated VPL will be validated using data derived from terrestrial planets in our own solar system. It will then be used to explore the plausi-

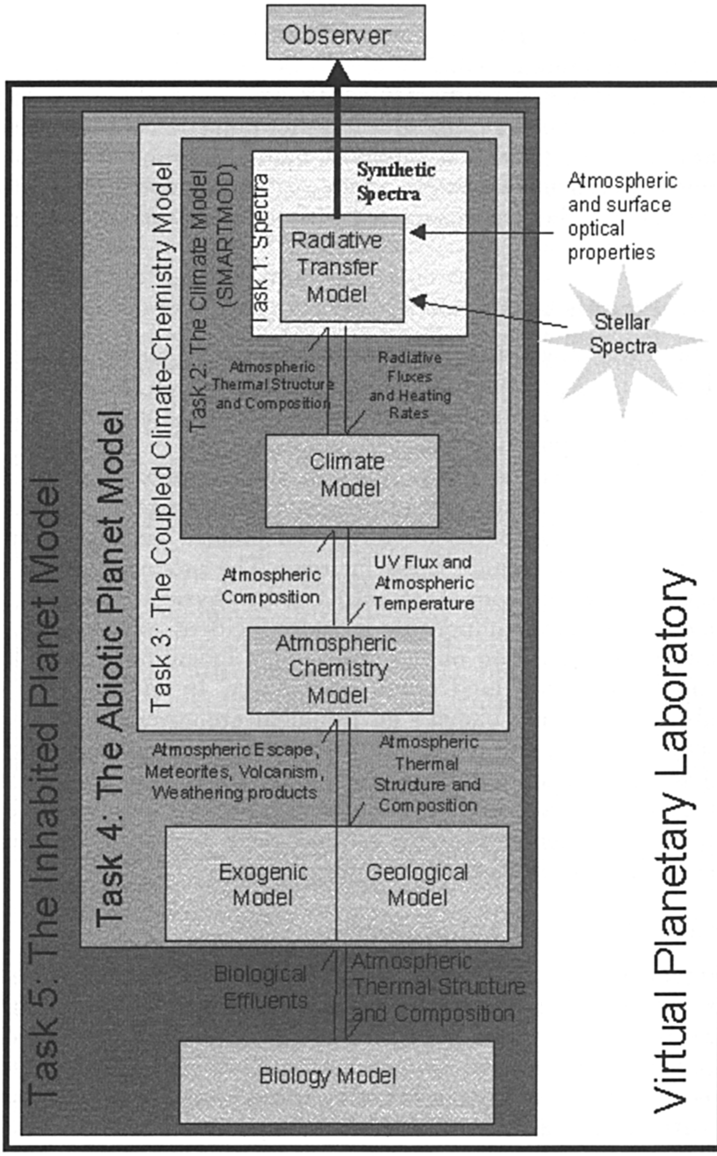

Figure 2. The suite of radiative transfer, climate, chemical, geological, and biological component models are shown as boxes, and their interactions with each other are shown by the arrows. The information transferred between these component models is labeled at each interface. The principal product at each Task development stage is a suite of synthetic spectra which can be used to identify potential biosignatures and derive required capabilities for astronomical instrumentation.

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ble range of atmospheric compositions and thermal structures, and to generate disk-averaged spectra for extrasolar planets and for early Earth. These models will be run with and without biological processes to improve our understanding of the effects of life on a planet's atmospheric composition and spectrum. They will also be used to create a spectral catalog that can be used as a statistical sample space to explore the optimum wavelength range, spectral resolution, and instrument sensitivity required to characterize extrasolar terrestrial planets.

Current work includes using a self-consistent coupled climate-chemical model, and a radiative transfer model to explore the change in the spectrum of an Earth-like planet as a function of oxygen abundance in that atmosphere. Figure 3 shows the changes throughout an optical/NIR/MIR spectrum when the oxygen abundance of an Earth-like atmosphere is severely depleted. Note that coupled changes due to the change in composition and the corresponding change in temperature structure produce effects that are more involved than a simple reduction in oxygen or ozone abundance.

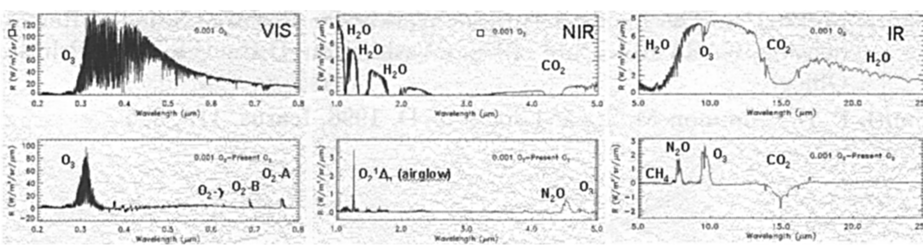

Figure 3. Difference spectrum generated by subtracting the spectrum of an Earth-like planet with the present atmospheric level (PAL) of oxygen, and an Earth-like planet that has one thousandth of PAL.

3. Conclusions

The characterization of terrestrial planets from around other stars is an emerging field that could gain a great deal from existing techniques and tools used by the Earth-observing and planetary science communities. These include remote-sensing techniques (atmospheric thermal structure and composition, land processes, clouds, aerosols, etc.) and environmental models, including atmospheric chemistry, climate, carbon cycle, hydrological cycle and biospheric models. These techniques and models can be used to provide a rigorous scientific basis for studies of the habitability and detection of life in a broad range of plausible planetary environments.

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