Jet Propulsion Laboratory (2)

Pasadena, California

Astronomical Detection of Biosignatures from Extrasolar Planets

Principal Investigator:

Victoria S. Meadows, Jet Propulsion Laboratory

Co-Investigators/Collaborators:

Mark A. Allen, Jet Propulsion Laboratory
Yuk Ling Yung, California Institute of Technology
Kevin Zahnle, NASA Ames Research Center
Thangasamy Velusamy, Jet Propulsion Laboratory
Michael C. Storrie-Lombardi, Jet Propulsion Laboratory
Mark Richardson, California Institute of Technology
Kenneth H. Nealson, Jet Propulsion Laboratory
James F. Kasting, Pennsylvania State University
Wesley T. Huntress, Jr., Carnegie Institution of Washington
David Crisp, Jet Propulsion Laboratory
Martin Cohen, University of California, Berkeley
Linda R. Brown, Jet Propulsion Laboratory
Cherilynn A. Morrow, Space Science Institute
Amir Fijany, Jet Propulsion Laboratory
Rob Rye, California Institute of Technology
Norman Sleep, Stanford University

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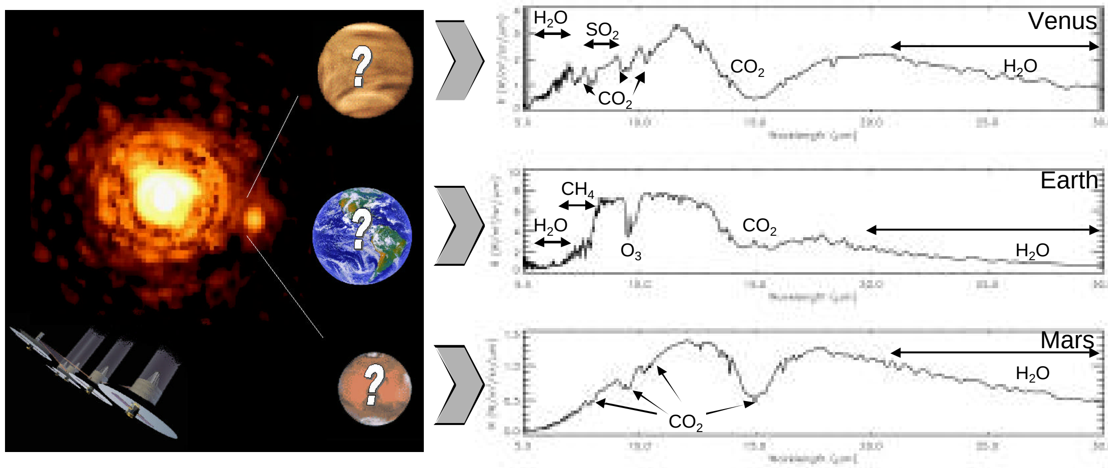
A.0 EXECUTIVE SUMMARY



Are we alone? The goals of the proposed research are to understand the plausible range of atmospheric and surface compositions for terrestrial planets, and to learn how to use spectra to discriminate between extrasolar planets with and without life. The results of this research will provide essential material to drive the instrument design and search strategies for future NASA extrasolar planet detection and characterization missions.

A.1 PROPOSED PROGRAM

A.1.1 RATIONALE

Motivated by the recent discoveries of a multitude of extrasolar planets, NASA has initiated a series of studies for space-based observatories that will be able to search for life on these worlds. To optimize the designs of these NASA missions and to ultimately interpret the data that they return we must have the capability to recognize habitable worlds and to discriminate between planets with and without life. The intent of the proposed modeling work is to learn how to recognize the presence of life on extrasolar terrestrial planets by identifying the signatures of life in their spectra.

A.1.2 INNOVATIONS

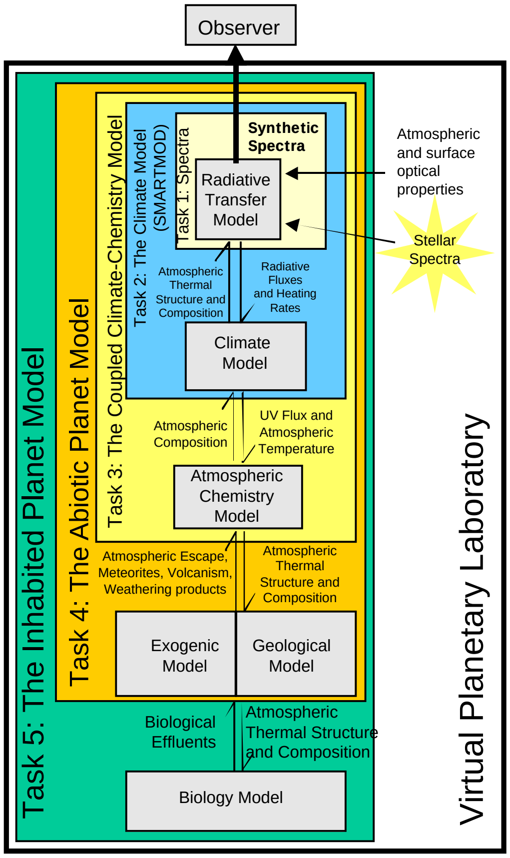
To achieve our goals we will develop a suite of innovative modeling tools to simulate the environments and spectra of extrasolar planets. These modeling tools will constitute a Virtual Planetary Laboratory and will provide the first models to couple the radiative fluxes, climate, chemistry, geology and biology of a terrestrial planet, to produce a self-consistent planetary state. This powerful new facility will generate of a wide range of plausible atmospheres for extrasolar planets, and for the atmospheres of early Earth.

A.1.3 DISTINGUISHING FEATURES

The proposed research is a significant multidisciplinary effort that combines existing models from five major research fields to develop a theoretical framework which parameterizes all the major processes of a terrestrial planet. The comprehensiveness and flexibility of the modeling tools enables a non-Earth-centric study of terrestrial planet atmospheres and the signs of life to extend our search for the signs of life to non-oxygen producing life, around stars very different to our own.

A.1.4 UNIFYING INTELLECTUAL FOCUS

Our objectives are to understand the characteristics and environments of plausible extrasolar planets both with and without life, and to use that understanding to drive the design and search strategies for future planet detecting and characterizing observatories.



The Virtual Planetary Laboratory

A.1.5 PROPOSED RESEARCH

The proposed research will provide improved understanding of the nature and characteristics of extrasolar planets, and the early Earth, and allow us to recognize the signs of life in these environments. This research will specifically address the question of “false positive” detections of life, and also help to quantify the effect of life on the atmospheric composition and spectrum of a terrestrial planet. The research tasks will ultimately provide a comprehensive spectral catalog, a "menu" of biosignatures, which will be used to determine the optimum wavelength range, spectral resolution and sensitivity required to remotely sense the signs of life in the atmosphere or on the surface of another world.

A.1.6 TRAINING PLANS

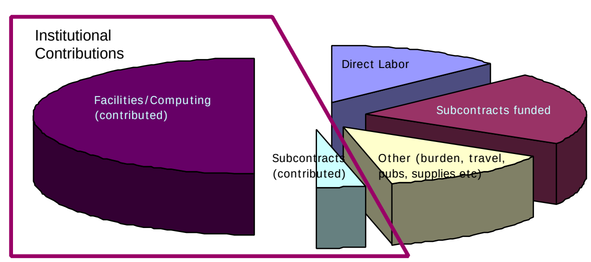
Training is an important part of this effort. Training is already in place for undergraduate and graduate students through the current education projects of its members. We will support 6 postdoctoral scholars with this effort and will train them in astrobiology and multidisciplinary research.

A.1.7 MANAGEMENT APPROACH OF PERSONNEL AND INSTITUTION

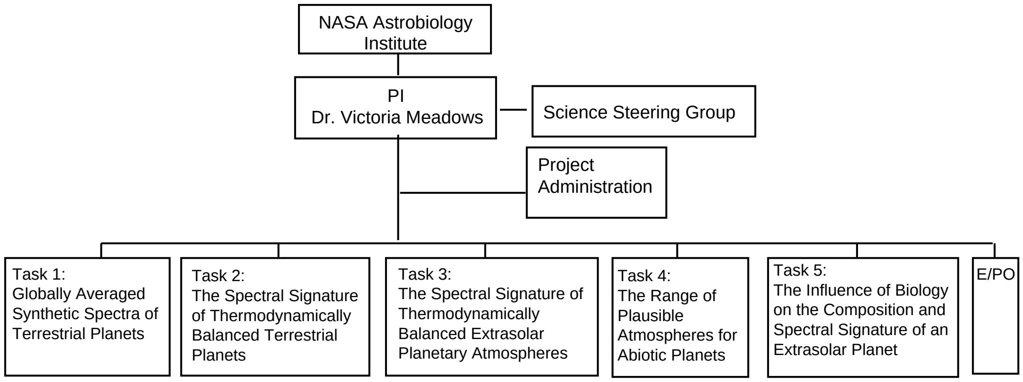
This research program is a cooperative effort consisting of a 17 member multidisciplinary team that leverages the resources and knowledge from 7 academic and research institutions. The majority of the computational research will be accomplished at JPL/Caltech, although all institutions will provide investigators' scientific expertise. Coordination and integration of the efforts of the research team members, in a timely manner, is the focus of this management activity.

The PI, Dr. Victoria Meadows, is accountable to NAI for the implementation, outcome, and scientific integrity of the research and the resulting products. The research efforts of the program will be accomplished within five major task groups, each with a Co-I task team and a Co-I assigned as Task Lead. A Science Steering Group, consisting of lead CoIs from five of the institutions, will assist the PI. The organizational structure also shows the EPO effort and the administrative support. The EPO effort will be managed in manner similar to the research tasks.

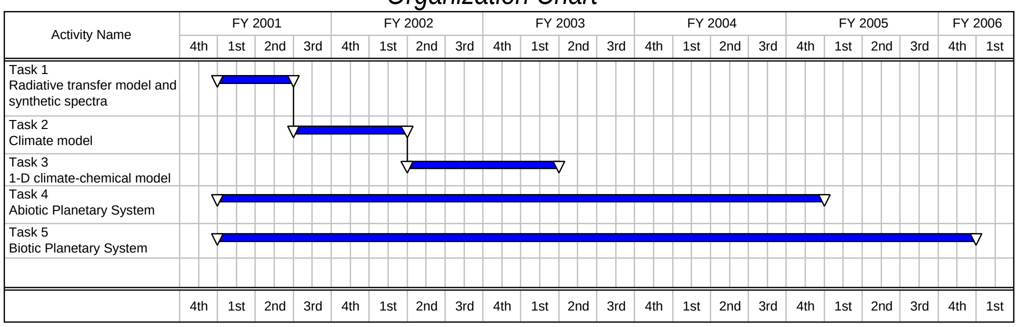
Tasks 1, 4 and 5 start in the first year of this effort. Task 1 starts the radiative-climate-chemical model development and Tasks 4 and 5 start by defining geological, exospheric and biological modules required for the planet models. Task 2 and 3 integrate climate and chemistry components to complete the mechanistic core of the planet models to be developed in Tasks 4 and 5. Work in the final two years of this effort will concentrate on integration of the geological, exospheric and biological modules with the mechanistic core to produce the planet models.



Funding Profile showing Institutional Commitments



Organization Chart



Schedule of Tasks

A.1.8 EPO ACTIVITIES

This proposal contains an Education/Public Outreach proposal. The EPO proposal uses the research proposal focus of developing methods to characterize and search for life on other worlds to offer a compelling context for learning fundamental concepts in Earth and space science, physical science and life science. This EPO plan will partner proposal scientists with education specialists to implement educator workshops and public symposia. We will also produce web resources that will prepare and follow up with workshop and symposia participants. These will include a low-resolution interactive version of the Virtual Planetary Laboratory being designed by the research team, and a "Family Guide" addressing the search for life on other worlds.

A.1.9 INSTITUTIONAL COMMITMENTS

This proposal has a strong institutional commitment. JPL will provide a significant commitment in the form of $5.2M of supercomputing facilities, as well as office space and administrative and budgetary support for the project. Five of our other team institutions will provide commitments in the form of salaries, office space and computational facilities for five of the Co-Is.

A.1.10 IMPLEMENTATION OF COLLABORATIVE AND NETWORKING CONCEPTS OF THE NAI

Our research program will also support NAI's annual integration workshop and we will participate in the preparation of workshop reports. All research products will be documented in the open literature and available for the NAI/scientific community for review. The Virtual Planetary Laboratory will be a valuable tool for enhancing our understanding in a broad range of astrobiology fields. The VPL will be developed in collaboration with three other NAI member institutions, and will ultimately be made available for collaborative use with other members of the NAI.

The Next Generation Internet (NGI) will be used heavily to manage the research activities outlined in this proposal. Since all CoIs are at or near institutions already having a NAI-supplied videoconferencing area, a large fraction of the Science Steering Group meetings and the Research Program Team Progress meetings will be held as videoconferences.

C.0 RESEARCH/TRAINING/MANAGEMENT

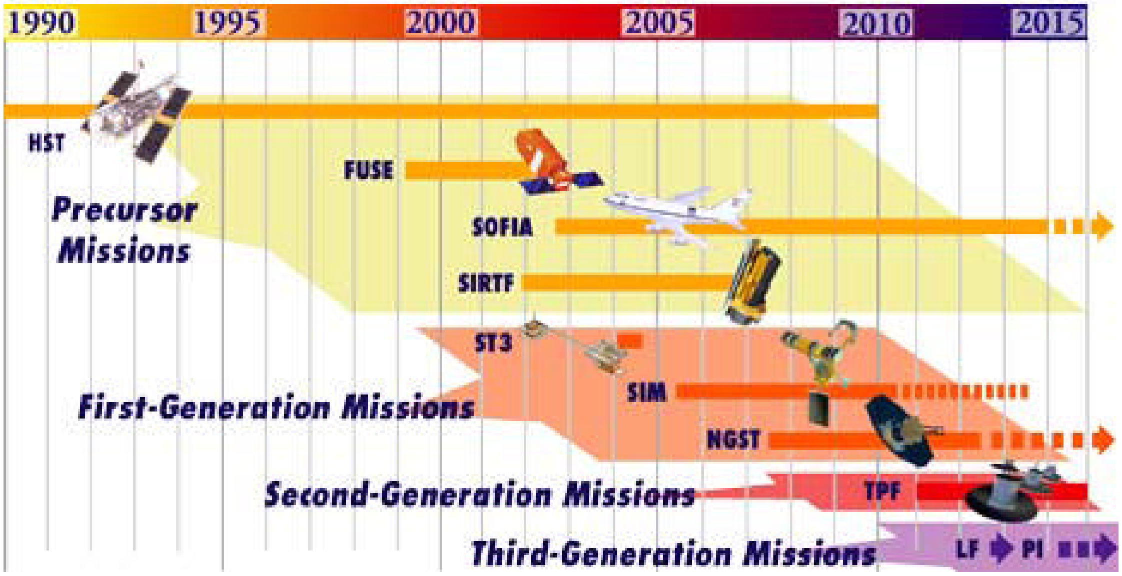


Figure C.1.1 Timeline of origins astronomical observing platforms (Origins Web site)

C.1 OBJECTIVES AND EXPECTED SIGNIFICANCE OF RESEARCH

The principal goal of this proposal is to learn to recognize biospheres on extrasolar planets by identifying the signatures of life that could be detected in their spectra (Goal 7 of the Astrobiology Roadmap, a preferred, currently underrepresented Roadmap goal).

Spurred by the recent discoveries of a multitude of extrasolar planetary systems, studies are already underway for instrumentation that can search for life on extrasolar planets, such as the space-based Terrestrial Planet Finder (TPF) mission, to be launched in 2011, and the next generation follow-on, the Life Finder mission. With these observatories currently in the early planning stages, our proposed work will provide timely resources and improved guidelines to better define the required capabilities and optimum survey strategies for these missions (Figure C.1.1).

To support these future missions, we will develop the ability to recognize habitable worlds and to discriminate between the spectra of planets with and without life.

We will also determine the optimum wavelength range, spectral resolution, and signal-to-noise ratio required to detect the signs of life on other planets.

C.1.1 WHAT IS AN ASTRONOMICAL BIOSIGNATURE?

Some of the most overt astronomical biosignatures (signs of life visible from space) on our own planet are spectral features indicating the presence of liquid H_2O and chlorophyll on the surface, and abundant oxygen in the atmosphere (Figure C.1.2).

However, some of these astronomical biosignatures have only been characteristics of the Earth's spectrum for about half the time that the Earth has supported life (Holland, 1994). 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 and 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.

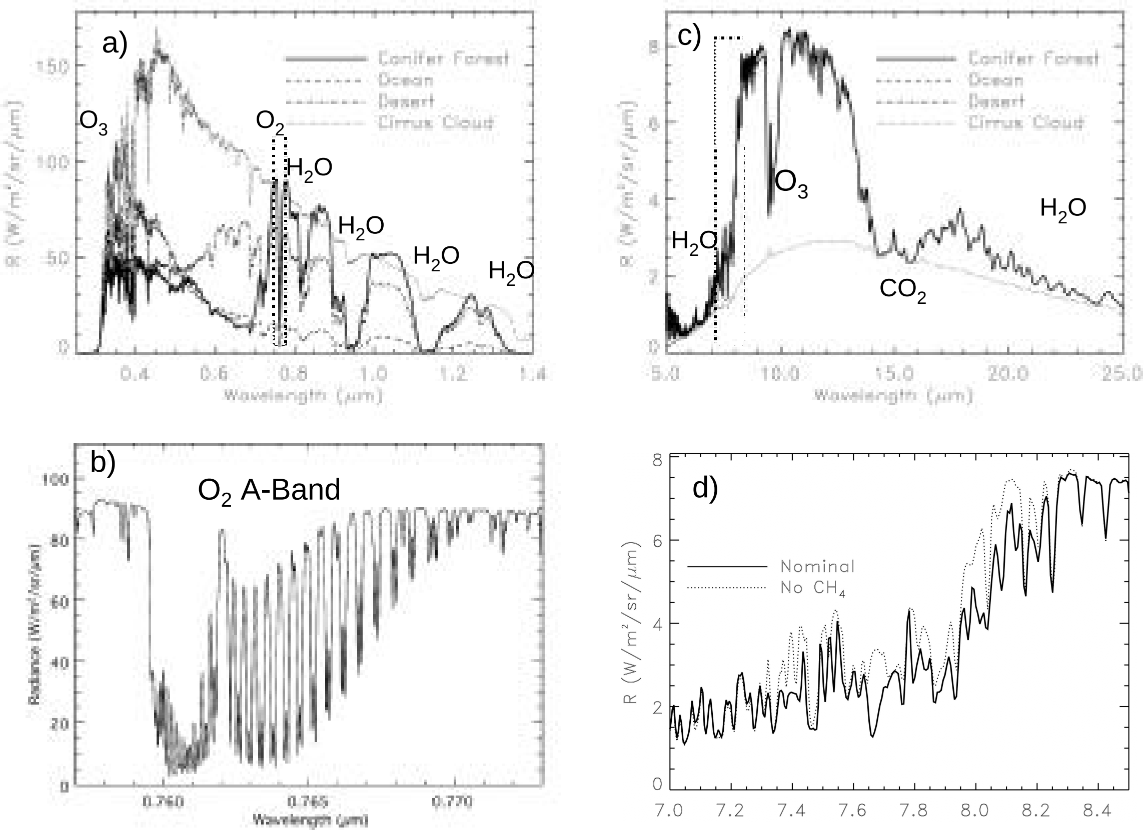


Figure C.1.2 The Earth's Biosignatures. Synthetic spectra of clear and cloudy terrestrial environments at solar (left) and thermal (right) wavelengths generated with the spectral mapping atmospheric radiative transfer (SMART) model. a) Synthetic solar reflection spectra of clear atmospheres over a conifer 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 and the atmospheric thermal structure and the abundance profiles for H_2O, CO_2, O_3, N_2O, CO, CH_4, and O_2 are from the McClatchy et al. (1972) mid latitude summer atmosphere. Chlorophyll, a potentially important biosignature, has strong absorption in the UV and blue (<0.5μm) and in the red (0.6-0.7 μm), slightly less absorption in the green (0.55 μm). It is also sunlight highly reflective just beyond the visible range (>0.7 μm). Ozone (<0.3 μm), water vapor, and the O_2 A-Band (panel c) are also prominent in the Earth's solar spectrum. However, high clouds can hide most of these features. c) 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 (panel d), but their spectral signatures are far more subtle than the biosignatures at solar wavelengths.

C.1.2 RESEARCH OBJECTIVES

To reach our goal of being able to recognize the signatures of life on extrasolar planets, we have developed a series of research objectives, which are described below. These research objectives will be achieved with our research tasks, which will provide the theoretical framework required to recognize biosignatures in the spectra of extrasolar planets and to provide recommendations for instrument capabilities and search strategies required to detect astronomical biosignatures on extrasolar planets.

OBJECTIVE 1: REQUIREMENTS FOR DETECTING ATMOSPHERIC AND SURFACE CHARACTERISTICS ON AN EARTH-LIKE PLANET

We will explore the sensitivity of astronomical instrumentation to globally-averaged surface and atmospheric properties, and astronomical biosignatures for modern-day Earth.

OBJECTIVE 2: EXTRASOLAR PLANET ATMOSPHERES AND THE DETECTABILITY OF BIOSIGNATURES

We will move beyond the Earth-centric study of biosignatures to determine plausible atmospheric and surface compositions for a range of different terrestrial planet types around stars other than our own Sun. The detectability of biosignatures from these extrasolar atmospheres and surfaces will also be studied. This study for detectability, and subsequent studies throughout the proposed work will focus on detectability of biosignatures over a broad spectral range from the UV to the far-IR, and for different types of astronomical instrumentation.

OBJECTIVE 3: EARLY EARTH ATMOSPHERES AND THE DETECTABILITY OF BIOSIGNATURES

We will determine plausible environments for various stages of the Earth's abiotic and inhabited early history. We will understand the spectroscopic appearance of these early Earths, and how to identify biosignatures in the inhabited environment using astronomical instrumentation.

OBJECTIVE 4: ABIOTIC PLANET ATMOSPHERES AND THE DETERMINATION OF FALSE POSITIVES

We will understand the range of planetary atmospheres possible on a terrestrial planet without life. This study will allow us to identify possible "false positives", planets without life that display spectral features that would otherwise be considered a biosignature. We will identify the circumstances under which a false positive can occur, and make recommendations on how to discriminate between a false positive signature and a true biosignature.

OBJECTIVE 5: INHABITED PLANET ATMOSPHERES AND THE DEFINITION OF NEW BIOSIGNATURES

We will explore the effects of life on a planetary atmosphere and determine new biosignatures for a range of different terrestrial planet atmospheres.

C.1.3 THE VIRTUAL PLANETARY LABORATORY

To achieve our research objectives we will develop a Virtual Planetary Laboratory (VPL), a suite of computer models that will allow us to simulate a broad range of planetary environments both with and without life, and to determine the spectral signature of these environments. These tools provide a significant innovation, because they will contribute completely new capabilities for understanding extrasolar planetary atmospheres and for astronomical biosignatures. These tools will be validated using observations of the current Earth's environment, with other terrestrial planets within our own solar system as controls. We will then realistically simulate the range of environments of the Early Earth and their spectra. To further expand our ability to recognize life on other planets we will ultimately generalize this effort to simulate biosignatures in terrestrial planetary environments very different from Earth around stars other than our own Sun.

Results generated throughout this multidisciplinary investigation will improve our understanding of the habitable zone (HZ) around other stars (Astrobiology Roadmap Objective 12) and will allow us to identify new potential biosignatures for a range of planetary environments other than that of present day Earth (Astrobiology Roadmap Goal 7 and Objective 13). The vast compendium of realistic synthetic spectra generated by this study will be analyzed to yield recommendations for required capabilities and optimum search strategies for future extrasolar planet detecting and characterizing instrumentation.

C.1.4 SIMULATING PLANETS AND THEIR SPECTRA WITH THE VIRTUAL PLANETARY LABORATORY

The spectrum of a planet is the product of the complex interplay of a broad range of environmental components and processes (Figure C.1.3). Hence, to generate realistic spectra of a range of plausible extrasolar terrestrial planets we must simulate planetary environments that include all the basic environmental components. 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)

Click here to see Figure C.1.3. Click on the figure to return back to here.

Figure C.1.3 Diagram demonstrating the basic components and planetary processes that ultimately contribute to the spectrum of a planet

The evolution and equilibrium state of a planet's environment are governed by a series of coupled physical, chemical, and biological processes. These processes are:

- 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
- life processes such as respiration and photosynthesis

The Virtual Planetary Laboratory will simulate these planetary components and processes by integrating a series of existing, rigorous, radiative-transfer, climate, and chemical models that are currently used for studies of planets in our solar system, with geological and biospheric models that will be developed during the course of this activity.

The synthetic spectra generated by these models will be analyzed using a suite of statistical tools and astronomical instrument simulators to provide recommendations for the required spectral resolution, wavelength range, and signal to noise ratio needed to detect life on extrasolar planets. Once validated and documented, the VPL will be made available to the Astrobiology community through a Web-based interface or collaboration with our team. This powerful and versatile tool has many potential applications beyond the scope of this current proposal, and we have already identified a number of potential uses by other NAI members. These include:

- derivation of plausible extrasolar atmospheric compositions that can be generated for laboratory tests on microbial evolution and adaptation, and
- providing a theoretical framework in which to model and visualize the NAI's ongoing work on geological and biological processes and their effects on plausible atmospheres for early Earth and extrasolar planets.

Construction of the VPL will be achieved through five tasks, where each successive task builds substantially on the work of previous tasks. This hierarchical implementation plan allows us to validate the model and produce interim results at each stage of added complexity and versatility. The major components of the VPL and their interrelationships are shown in Figure C.1.4. Note that this proposal is principally a computer modeling task. No new instruments or hardware are needed to achieve our stated objectives.

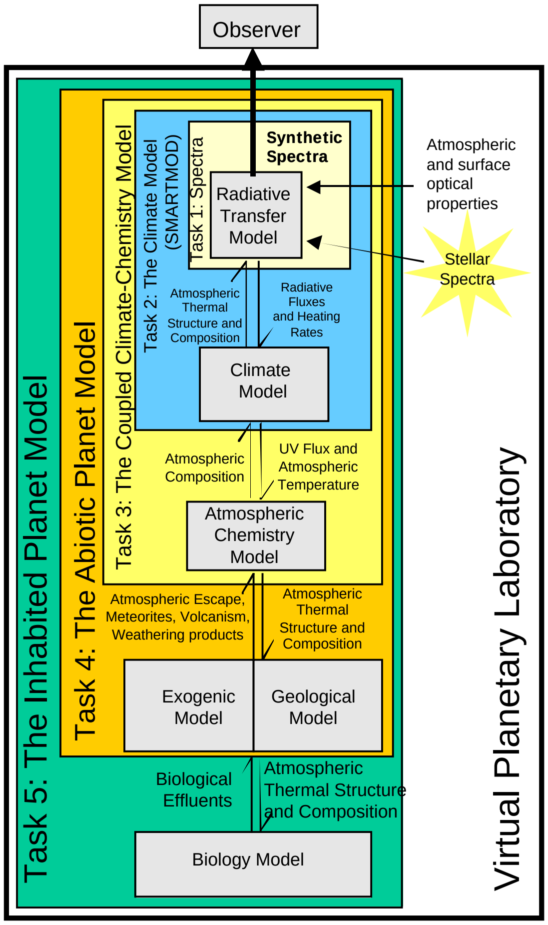


Figure C.1.4 This diagram shows the structure of the Virtual Planetary Laboratory. The suite of radiative transfer, climate, chemical, geological, and biological component models are shown as boxes, and their interactions with each other are shown by the arrows. The information transferred between these component models is labeled at each interface. The order in which these component models are coupled to each other during the course of this proposed work is specified by the Task number. 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.

C.1.5 RESEARCH TASKS

To address our goals and objectives, the proposed research is divided into five tasks. With our final task, we will have developed a suite of tools for modeling biosignatures that will provide a significant improvement over currently available models. We will also provide improved understanding of plausible extrasolar and paleoatmospheres, and biosignatures and their detectability over a broad wavelength range applicable to many different astronomical technologies. The five tasks and the research objectives they address are:

- Task 1: Globally averaged synthetic spectra of terrestrial planets (Objective 1)
- Task 2: The spectral signature of thermodynamically balanced terrestrial planets (Objective 2)
- Task 3: The spectral signature of chemically and thermodynamically balanced extrasolar planetary atmospheres (Objectives 2 and 3)
- Task 4: The range of plausible atmospheres for abiotic planets (Objectives 2, 3 and 4)
- Task 5: The Influence of Biology on the Composition and Spectral Signature of an Extrasolar Planet (Research Objectives 2, 3, 4 and 5)

The first three tasks will also indicate the best wavelength range and spectral resolution for detecting the bulk atmospheric composition, physical properties, and trace gas abundances for a range of plausible atmospheres and for a number of different parent stars. The final two tasks will culminate in the development of coupled radiative and chemical models, with geological and biological processes, to determine the chemical equilibrium state for terrestrial planets with and without life. The atmospheres generated in this task will be visualized by tools developed in the second and third tasks, and the synthetic spectra of inhabited planets generated by this task will be used to identify new potential biosignatures.

To execute these tasks and develop the Virtual Planetary Laboratory, we require expertise in atmospheric photochemistry, atmospheric radiative transfer, molecular spectroscopy, climate modeling, paleoatmospheres, geochemistry, oceanography, and stellar spectral energy distributions. We also require plausible constraints on the sources and sinks of abiotic volatiles (impacts, volcanism, tectonics), as well as the sources and sinks of biogenic gases and biogenic surface signatures. Finally, the sophisticated modeling tools required to simulate these processes also necessitate high-speed computing.

To provide this expertise, we have assembled a multidisciplinary team of 17 experts from 7 institutions. This team and their roles are described in detail in the management plan.

C.1.6 SIGNIFICANCE OF THE PROPOSED WORK AND ANTICIPATED PRODUCTS

Much of the existing research in astrobiology focuses on the detection and recognition of the signs of life using *in situ* techniques to search for life on the surface of bodies in our own solar system.

This research will take the search for life beyond the confines of our own solar system and will provide a solid foundation for a new research field which has been identified as an underrepresented Astrobiology Roadmap Goal.

This work will provide the first systematic exploration of plausible atmospheres and conditions on extrasolar planets. In doing so, we will provide additional insight into the extent of the habitable zones around a range of stellar types. It will also elucidate the range of equilibrium atmospheric compositions that are associated solely with abiotic processes. Comparisons between an abiotic planetary model and a planetary model with life will allow us to assess the effects that life has on a planetary atmosphere, and to identify potential new biosignatures for a range of plausible extrasolar planet atmospheres and surfaces.

The principal product of the proposed work will be an improved understanding of the detectability of biosignatures in the a broad range of planetary environments. This effort will also produce a suite of powerful and versatile computer models that can be accessed by the Astrobiology community to run a wide range of experiments. The results of this research will provide a comprehensive spectral catalog, a "menu" of biosignatures, and recommendations for instrument capabilities for the development of missions that seek to detect life on other planets using astronomical techniques.

C.2 HOW THIS WORK WILL BUILD ON AND EXTEND THE STATE OF KNOWLEDGE

With this proposed work, we will provide a solid theoretical foundation for a field that is currently in its infancy. We will address the shortcomings that exist in the current models being used to study the detectability of biosignatures, and we will provide improvements in modeling methods, inputs and computational efficiency. We will also expand the existing modeling studies to cover a broad range of wavelengths, and include non-oxygen producing life, on planets other than Earth, around stars other than our Sun. In so doing we will improve our understanding of extrasolar planets, and provide the rigorous and comprehensive modeling work required to support and guide every step of the observational process for detecting biosignatures in extrasolar planets.

C.2.1 IMPROVEMENTS IN MODELING

Existing studies of the detectability of astronomical biosignatures are extremely limited. Preliminary work on this topic can be found in the many feasibility studies for the Terrestrial Planet Finder mission (TPF book), and in conference proceedings for the NAI sponsored Pale Blue Dot Workshops (e.g. Traub and Jucks, 2000).

However, the most comprehensive paper on this topic published in a refereed journal is that of Schindler and Kasting (2000). To support the design of TPF-like instruments, these authors calculated synthetic thermal-IR spectra of oxidizing atmospheres containing various amounts of O_2 (and hence, O_3) and of reducing atmospheres containing various amounts of CH_4. They found that atmosphere containing more than about 1% of the present atmospheric level (PAL) of O_2 should have a detectable ozone signal for a high-resolution TPF, while atmospheres containing more than about 100 ppm of methane should have a detectable CH_4 signal.

These calculations were not, however, performed in a fully self-consistent manner. In the O_2/O_3 calculations, the temperature bulge in the stratosphere caused by heating by O_3 was simply removed for calculations at lower O_2 levels. In the CH_4-rich, primitive atmosphere calculations, stratospheric heating by CH_4

(which absorbs visible and near-IR solar radiation) was neglected. Incorrect estimates of the resultant temperature structure can affect the detectability of trace gases. Thus, these calculations are suggestive of what atmospheric biosignatures might be present, but they need to be redone with more self- consistent models.

Previous models used for these studies also have other shortcomings, which include:

- Limited spectral range (solar and near infrared wavelengths neglected)
- Multiple scattering by clouds and aerosols is not treated realistically, or neglected entirely
- Except for the present-day Earth cases, the chemical composition of the atmospheres are not self-consistent
- Spectra have been generated for isolated atmospheric profiles, neglecting spatial gradients in temperature or optical properties that might affect disk-averaged measurements.
- The effects of attenuation by zodiacal dust and limitations in instrument performance (spectral resolution, spectral range, and signal to noise) are not considered.

Models developed by this research effort as part of the Virtual Planetary Laboratory will overcome all the above shortcomings to derive plausible extrasolar atmospheres that are radiatively, physically, and chemically self-consistent.

C.2.2 EXPANDING THE WAVELENGTH COVERAGE

Existing work on the detectability of astronomical biosignatures has also focused principally on a narrow region of the mid-infrared. This focus on mid-infrared wavelengths was driven by initial designs for missions like Terrestrial Planet Finder, which are 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 may provide sufficient suppression of light from the parent star that they could also be feasible within the TPF time frame-generation. Coronagraphs could therefore provide a means to search for biosignatures over a promising spectral range for which there are few if any focused studies on their detectability.

To improve our understanding of potential biosignatures and their detectability throughout the spectrum, we therefore need to attack on two fronts. First, we need to better understand the features available in the mid-infrared region for a range of plausible extrasolar planets, not just for the commonly-modeled clear-sky Earth. Secondly, we need to comprehensively explore biosignatures available at other wavelengths that may be accessible to technology different than that currently planned for TPF.

C.2.2.1 FURTHER WORK REQUIRED IN THE MID-IR

If nulling-interferometery is chosen as the observing technique for TPF, then clearly we need to rigorously model the mid-IR spectral region for a range of plausible extrasolar planet atmospheres to determine:

- Sensitivity to known mid-IR biosignatures for a range of different trace gas abundances and bulk atmospheric composition (Figure C.1.2d)
- Sensitivity (if any) to surface biosignatures (Figure C.1.2c)
- Potential new biosignatures for a range of paleo-Earth atmospheres and sensitivity to these biosignatures
- Potential new biosignatures for a range of atmospheric types other than that of present day or paleo-Earth and sensitivity to these biosignatures
- Potential sources of spectral confusion due to overlapping features from other molecules
- The effect of clouds on the detectability of biosignatures (Figure C.1.2c)
- Potential "false positives" in this wavelength range. Spectral signatures that mimic those produced by life, but are instead derived from an abiotic source in the planet's atmosphere or on its surface
- Improved estimates for S/N, spectral resolution, and optimum wavelength range for robust detection of biosignatures

All this information will be provided by the Virtual Planetary Laboratory over the course of our proposed work.

WHY WE SHOULD EXPLORE WAVELENGTHS OTHER THAN THE MID-IR

In addition to exploring the 5-30μm region in more depth than existing studies have done, there are many reasons to explore wavelength regimes beyond this region.

Enhanced Detection of Disequilibrium Biosignatures: The mid-IR region is not optimal for detection of classic disequilibrium biosignatures (like CH_4 or N_2O in the presence of O_2) These features are much more obvious at optical and near-infrared wavelengths, as already demonstrated during the Galileo flyby of Earth (Sagan, et al 1993). These disequilibrium biosignatures are likely to be more robust indicators of life, and desirable targets for the next generation of planet detection and characterization missions. 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 and 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 higher than R=1250 because the absorption features are strongly overlapped (Figure C.1.2d).

Sensitivity to Surface Features: As is graphically demonstrated in Figure C.1.2c, 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 mainly 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 Figure C.1.2a the optical and near-infrared regions of the spectrum display a rich array of spectral features due to 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.

Although current technology still favors the mid-infrared region for observing extrasolar terrestrial planets, more robust indicators of habitability and life may be available in other spectral regions. The detailed study proposed here, which will explore planetary features and biosignatures available over a broad wavelength range will allow us to identify the best wavelength choices for determining the atmospheric and surface characteristics of a planet, including the presence of life. The proposed work will also allow us to make an informed decision as to whether more robust biosignatures in other wavelength regions compel us to develop the more challenging technology required to observe terrestrial planets at optical and near-IR wavelengths.

C.2.3 DETERMINING FALSE POSITIVES

Early TPF support studies indicated that the presence of ozone may be the best biosignature available in the targeted mid-IR region. Angel et al, (1986) first pointed out the significance of ozone as a potential biosignature. Unlike O_2, O_3 absorbs in the thermal IR, with a strong band at 9.6um. In the Earth's atmosphere ozone has a nonlinear dependence on the atmospheric O_2 abundance. Models indicate that it rises to appreciable concentrations even at relatively low O_2 levels (Kasting and Donahue, 1980). Hence, the presence of ozone, and the consequently inferred presence of oxygen, while being highly suggestive, and an excellent first step target, is not on its own an unambiguous or comprehensive indicator of life.

There are several known mechanisms by which oxygen can be produced abiotically in a planet's atmosphere. These include photodissociation of water vapor on modern day Earth, and potentially during the loss of Venus' ocean in its early history (Schindler and Kasting, 2000), photodissociation of CO_2 (on present day Venus and Mars), and reduction of the normal planetary sinks for oxygen on small planets that lack volcanism and weathering (Mars).

To guard against misinterpreting spectra of extrasolar planets, we will use the VPL to better understand the plausible atmospheres likely for terrestrial planets that do not contain life, and to understand under what conditions an abiotic planet could mimic a biosignature (i.e. produce a "false positive"). In the course of this study, we will also be able to determine any auxiliary information needed to distinguish between abiotic or biological sources (such as planet size, planet-star separation, and the presence of other gases in the spectrum).

C.2.4 EXPANDING THE TYPES OF LIFE AND THEIR ENVIRONMENTS

Current studies of the definition and detectability of astronomical biosignatures have also concentrated almost exclusively on biosignatures for life that produced oxygen, on a planet orbiting a star with the same spectral characteristics as our own Sun. A search for life that is targeted principally on oxygen-producing life may fail to recognize planets that are inhabited by organisms that produce different biogenic gases like those produced by early life on Earth. However, even though we are developing an understanding of the biology and chemistry of this early life, the atmospheric and surface signatures of this form of life are not fully understood.

Similarly, the climate and atmospheric temperature structure of a planet's atmosphere is strongly affected by the spectrum of radiation output by the parent star. Assumptions made about the detectability of biogenic gases may no longer be valid when dealing with a planet orbiting a star of very different spectral type than our own, with a different atmospheric temperature structure and reflected stellar spectrum.

With the proposed work we will expand upon existing work to consider different forms of dominant carbon-based life on a planet's surface, and will the understand the chemistry and climate of planets orbiting stars other than our own.   These studies will greatly expand the likelihood of recognizing life on a wider variety of extrasolar planets.

C.3 TECHNICAL APPROACH AND METHODOLOGY

To achieve our research objectives, we propose an innovative, comprehensive, systematic, multidisciplinary modeling study. This research program will consist of 5 major modeling tasks. These 5 tasks allow us to progressively build a suite of models into a tool that we call the Virtual Planetary Laboratory (VPL). We will use the VPL to derive plausible surface and atmospheric environments for extrasolar planets, and generate high-resolution spectra of the radiation that they reflect and emit. These spectra will be studied to discover and characterize new astronomical biosignatures. This work will help drive the design and search strategies for planet detecting and characterizing instrumentation.

Once completed and validated, the VPL will be made available to the community as a multipurpose tool. This tool will be able to assimilate ongoing research on geological and life processes from members of the NAI and visualize the effect of our new understanding on the atmospheric composition and spectral signature of a terrestrial planet.

The VPL will incorporate a set of existing, highly sophisticated radiative transfer, climate, and chemical models that were developed and validated for studies of the atmospheres of the Earth and other planets in our solar system. These component models provide significant improvements over those that have been used in earlier astronomical biosignature studies. The combined model will contribute completely new capabilities for defining and detecting astronomical biosignatures.

Each of our 5 research tasks will incorporate the tools developed in all previous tasks, and will include a series of experiments to validate and utilize the integrated product. This approach is illustrated in Figure C.1.4. In each step, the number of parameters that must be specified a-priori will be reduced, as more processes are included explicitly in the models.

Task 1, Globally Averaged Synthetic Spectra of Terrestrial Planets: The objective of the first task is to understand the information content of disk-averaged spectra of terrestrial planets. To do this, we will use a radiative transfer model and atmospheric and surface data for Earth, Mars, Venus and Titan to generate spatially resolved synthetic spectra. These spectra will then be spatially averaged to simulate a range of illumination conditions (phase angles) and viewing geometries. These results will be processed with an observing system simulation tool, that simulates the spectral and spatial resolution, signal levels, noise sources, and other properties of planned space-based observing systems, including nulling interferometers and coronographs.

Our radiative transfer modeling tools have a number of advantages over those used in the pioneering studies of astronomical biosignatures by Schindler and Kasting (2000), Traub & Jucks (2000) and others. Specifically, our spectrum-resolving (line-by-line) model provides an explicit treatment of solar and thermal radiation in realistic, planetary atmospheres, where both gas absorption and multiple scattering contribute to the radiation field. Terrestrial spectra will be derived for a range of surface cover types (ocean, desert, grassland, bog, forest) atmospheric and surface temperature distributions, cloud cover, and trace gas abundances. Spectra of Venus, Mars, and Titan will be produced as abiotic controls. These results will be analyzed with instrument simulators to quantify the instrument parameters required to detect known biosignatures in the Earth's atmosphere, over a spectral range from the UV to the far-IR.

Task 2, The Spectral Signature of Thermodynamically Balanced Terrestrial Planets: One limitation of the methods described in Task 1 is that they require a significant amount of information about the physical and chemical properties of the planetary environments to be investigated. Environmental properties that contribute to the spectra of a terrestrial planet include the range of surface types and their areal coverage, the atmospheric thermal structure and composition, presence and spatial coverage by condensate clouds and photochemical aerosols, stellar illumination intensity and distribution, etc (Figure C.1.2). These methods are therefore best suited for studies of planetary environments whose physical and chemical properties are well constrained by observations. A broader range of environmental conditions can be used, but their properties must be specified a-priori, and substantial care is needed to insure that the combination of conditions is physically and chemically plausible.

In this task, we will develop realistic physical models to simulate environments that are roughly in physical, chemical, and biological equilibrium, such that they require a minimum number of ad-hoc parameters. This approach to an investigation of biosignatures is consistent with the conjecture that life can be detected as a thermodynamic and/or chemical process that forces environment conditions away from their abiotic equilibrium. Tasks 2 through 4 provide the tools needed to simulate equilibrium abiotic environments. Task 5 then introduces biological processes that perturb these environments, producing new equilibrium states whose spectra can be investigated to identify biosignatures.

In Task 2, a one-dimensional (1D) Radiative-Convective-Equilibrium (RCE) climate model will be used in conjunction with an energy balance climate model to construct a range of planetary environments that are thermally self-consistent with their prescribed chemical composition. Methods described in Task 1 will then be used to study their spectral signatures.

1D RCE climate models have been widely used for studies of the Earth (Manabe and Wetherald, 1967) and other planets in our solar system (Pollock et al. 1980; Crisp, 1989; Gierasch & Goody, 1968). These models provided valuable insight into the physical processes that control the thermal structures of these planets. They have also been used to simulate the paleoclimates of these atmospheres (Kasting, et al, 1984; Pavlov et al. 2000). However, they have not yet been used widely for studies of plausible extrasolar planet atmospheres.

The 1D RCE model adopted here also has several advantages over those used in earlier studies because it employs the comprehensive radiative transfer models described in Task 1, and includes a more realistic treatment of convection, condensation, and other physical processes. This model will first be validated through simulations of the current environments of Venus, Earth, Mars, and Titan. This validation exercise will include both comparisons of the equilibrium thermal structures of these environments and detailed comparisons of their reflected solar and emitted thermal spectra. The information content of the globally averaged, radiative equilibrium spectra generated for these bodies will also be compared to that of the spatially resolved and disk-integrated spectra of these terrestrial planets that were generated in

Task 1.

Task 3, The Spectral Signature of Chemically and Thermodynamically Balanced Extrasolar Planetary Atmospheres: In the third task, we will add even more to the range of realistic environments that can be investigated for the detectability of Earth's paleoatmospheres and biosignatures by generating spectra of extrasolar planets atmospheres that are in thermodynamic and chemical equilibrium with specified surface and exogenic boundary conditions. These environments will be simulated combining the 1D RCE climate model with an existing 1D photochemical model. With this combined model, we will explore the detectability of the currently accepted list of potential biosignatures in both oxidizing and reducing atmospheres, over a broad wavelength range, and for a range of stellar types. The high-resolution solar and thermal spectra generated in these experiments will be used to further constrain the instrument parameters and capabilities needed to retrieve the physical and chemical properties of these environments from whole-disk observations of extra-solar planets.

Task 4, The Range of Plausible Atmospheres for Abiotic Planets: The range of environments that can be studied with the models developed in the three Tasks is still somewhat limited, because ad-hoc surface and exogenic boundary conditions are still needed. The relevant surface boundary conditions include sources and sinks of volcanic effluents (gases and aerosols), surface weathering processes, and the exchange of volatiles between the atmosphere, land, ocean, and the planet interior. Exogenic processes that define the upper boundary conditions of the system (along with the incoming stellar flux and outgoing thermal flux) include the influx of meteoritic material and atmospheric loss.

Mechanistic models for these processes will be incorporated into the global 1D chemical/climate model in Task 4, to produce a versatile, self-consistent tool for simulating a broad range of abiotic planetary environments, and the spectra that they produce. (The Abiotic Planet Model). This model will first be validated through simulations of the present-day environments of Venus, Mars, and Titan. It will serve as the testbed for interdisciplinary studies of the plausible range of climate and chemistry for extrasolar terrestrial planets and for implications the habitability of these planets. We will use these results to determine likely "false positive" detections of life from abiotic planets. These studies will also include investigations of the equilibrium surface and atmospheric conditions of the abiotic early Earth, and early Mars and Venus, as well as a range of other highly oxidized and reducing environments with a range of surface and exogenic inputs.

Task 5, The Influence of Biology on the Composition and Spectral Signature of and Extrasolar Planet: As the final step in our effort to simulate the effects of life on extrasolar planets, we will incorporate a mechanistic model of a biosphere into the abiotic planet models developed in tasks 1-4. The biosphere model will modify the surface boundary fluxes of volatile species. This comprehensive, coupled, 1D climate, chemical and biological model (The Inhabited Planet Model) will be used to derive the age-dependent thermodynamic and chemical characteristics of planetary atmospheres and surfaces for a range of plausible biological inputs. At this point the IPM will support studies of the unique attributes of a habitable terrestrial-type planet that result from the presence of life, and the detectability of these attributes by remote-sensing spectroscopic observations. This will allow us to identify potential new biosignatures. The IPM will also provide insight into the possible ways that life can sustain the habitability of a planet.

Why Not Use a 3D Model? An important aspect of the VPL is the decision to use a one-dimensional framework. 3D models of the terrestrial climate system could be used as the basis for a generalized climate model. However, we believe that uncertainties in the application of these models to other systems, the vast increase in computational expense and complexity resulting from the use of these models, and the ability to constrain the key predictions resulting from such models (such as pole-to-equator temperature contrast, and species mixing) mean that application of a 3D framework at this stage is unnecessary-and indeed limiting.

Several factors compromise the utility of 3D tools for modeling the climates and biosignatures of extrasolar planets. First, even though the very best of these models do a very good job of simulating the Earth's present climate, they have been much less successful at modeling the circulation and spatially-dependent thermal structure of other planets. Specifically, these models have not yet been proven able to simulate the dynamics of planets with rotation rates that are slower (Venus) or faster (Jupiter, Saturn) than those of Earth. These shortcomings have been attributed to both the physics (vertical distribution of solar and thermal energy, treatment of free and forced convection, surface friction, *etc*.), numerics (numerical diffusion and dispersion, resolution) as well as the inherent assumptions made in these models (*e.g.* the Phillips thin atmosphere approximation, hydrostatic approximation, *etc*.). While there has been some recent progress on the slow and rapid rotation limits (*e.g.* Del Genio and Zhou, 1996; Showman and Dowling, 2000), these models have not yet been fully validated even for the easier problem of dynamics and the related pole-to-equator temperature contrast, let alone the more difficult problem of species transport.

The primary advantage of a mature and validated 3D circulation model would be its ability to self consistently determine the heat and species transport from system parameters such as the rotation rate, gravity, and surface properties (albedo, topography, etc.) Ultimately, such a modeling system should be developed to refine calculations undertaken with the Abiotic Planet Model. However, in most cases of yet-to-be-discovered extrasolar terrestrial planets, we will not have access to these important input parameters. For the APM, we will use prescriptions for the pole-to-equator temperature contrast and mixing which are based upon eddy parameterizations and/or global entropy considerations. While these parameterizations will be just as limited by the lack of input data and likely (at least) as erroneous in predicting mixing, they allow mixing to be treated as a free parameter for each case and allow vastly more APM experiments to be undertaken for a given amount of computing time. In short, the results of 3D calculations would not be significantly more rigorous, accurate, or dependable than ones derived using ad-hoc assumptions of these properties, based on observations of planets in our solar system.

The following 5 sections describe each task in greater detail. In each section, we will review the background and previous work pertinent to that task. We will also describe the technical approach (models), the research methodology, and the expected significance and products.

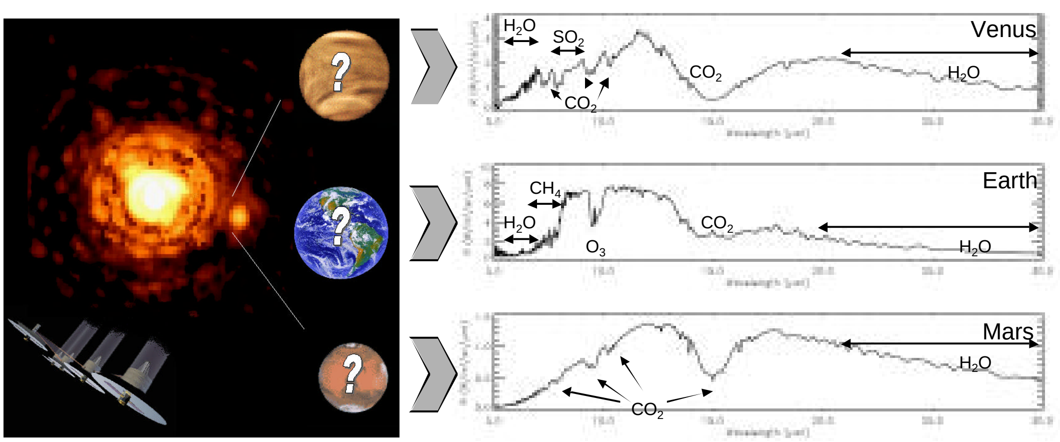


Figure C.3.1 Moderate-resolution spectra can be used to probe the atmosphere and surface of an extrasolar planet. Synthetic thermal IR spectra of Venus (top), Earth (middle), and Mars (bottom) obtained from the Spectral Mapping Atmospheric Radiative Transfer (SMART) model are shown at a resolution of 5 cm^{-1}. These spectra show the major absorption features in the CO_2-dominated atmospheres of Venus and Mars, and those in the $H_2O/CO_2/O_3/CH_4$ dominated terrestrial atmosphere. The CO_2 hot band at 9.4 μm overlaps the ozone 9.6 μm band, reducing its detectability in CO_2 atmospheres.

C.3.1 TASK 1: SENSITIVITY TO ENVIRONMENTAL PROPERTIES IN GLOBALLY-AVERAGED SYNTHETIC SPECTRA OF TERRESTRIAL PLANETS.

Spectroscopy is the most powerful technique available for retrieving the characteristics of planetary surfaces and atmospheres by remote sensing. 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 (Figure 1). 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. The objective of this task then is to understand the information available from disk averaged spectra of terrestrial planets. To do this, we propose to implement a suite of realistic atmospheric radiative transfer models and observational system simulation tools. The radiative transfer models will be used to generate high spectral resolution, spatially resolved spectra of the Venus, Earth, Mars, and Titan (Figure C.3.1). These spectra will then be averaged over the planet,s disk, and then processed with the observational system simulators to provide a quantitative assessment of their information content.

The following sections summarize the types of information that can be retrieved from the spectrum of a planet. We then describe the radiative transfer algorithms, their data requirements, and the observational system modeling tools adopted for this investigation. The role of ultracomputing is then defined and justified. Finally, we summarize the specific experiments and products, and their significance.

C3.1.1 WHAT CAN WE LEARN ABOUT AN EXTRASOLAR PLANET FROM DISK AVERAGED REMOTE-SENSING SPECTROSCOPY?

Remote sensing spectroscopy has provided the primary tool for documenting the properties of the surfaces and atmospheres of planets and their satellites in our solar system. This experience suggests that disk-averaged observations of an extrasolar planet can yield information about the following properties:

- The presence of an atmosphere and its bulk chemical composition
- The nature of the emitting/reflecting layer (solid/liquid surface vs. an opaque cloud deck) and its wavelength-dependent optical properties (albedo, thermal emissivity, temperature)
- Atmospheric pressure at the surface (or over an opaque cloud deck) and total atmospheric mass above that surface
- Atmospheric structure (variation of temperature and pressure with altitude).
- Trace gas mixing ratios and their spatial distribution.

Astronomical Biosignatures

In addition to the basic parameters described above, which are common to all planets with atmospheres, a planet which harbors life may also exhibit astronomical biosignatures, that is, spectral features that are indicative of life.

The concept of an astronomical biosignature was introduced as early as 1965 when James Lovelock proposed that the presence of chemically based life on a planet would change the composition of its atmosphere away from the abiological steady state, and that the change would be recognizable even at astronomical distances (Lovelock, 1965; Hitchcock and Lovelock, 1966). Lovelock went further to argue that on Earth at least, the interaction between life and the atmosphere was so intense, strongly driving our atmosphere away from the chemical equilibrium state, that the atmosphere could be regarded as an extension of the biosphere (Lovelock and Watson, 1982). If this is generally the case, studies of a planetary atmosphere should provide valuable clues to the presence of otherwise undetectable life on the planet's surface.

Lovelock also identified what is now perhaps considered to be one of the most conspicuous astronomical biosignatures, the simultaneous presence of an oxidized gas, such as O_2, and reduced gases such as CH_4 and N_2O at their present concentrations in the Earth's atmosphere. Earth's O_2 and CH_4 are in violation of the rules of (abiotic) equilibrium chemistry by orders of magnitude (Lovelock and Margulis, 1974). This disequilibrium pair can be detected via remote-sensing spectroscopy, given adequate spectral resolution and signal-to-noise, as was successfully demonstrated during the flyby of Earth by the Galileo spacecraft en route to Jupiter (Sagan et al., 1993).

The instrument on board Galileo that detected this biosignature was the Near- Infrared Mapping Spectrometer (NIMS), operating at 0.7

to 5.2 microns. Within that wavelength range, with a modest spectral resolution (λ/Δλ) of no more than ~100, NIMS was able to detect and quantify CO_2, CH_4, H_2O, O_2 and N_2O. The Galileo Ultraviolet Spectrometer (UVS) was also able to put a limit on the abundance of O_3.

In Task 1, we will undertake the first systematic exploration of sensitivity to changes in atmospheric and surface properties and the detectability of biosignatures in the globally averaged spectrum of the Earth's atmosphere. High-resolution synthetic spectra will be generated for a range of conditions, and then averaged over the disk from a range of viewing geometries to mimic what Earth would look like to the first (and probably second) generation extrasolar terrestrial planet detection missions. Similar results will be derived for Venus, Mars, and Titan, which will serve as abiotic controls.

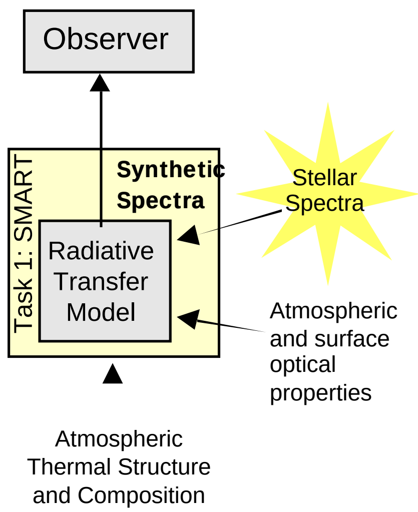


Figure C.3.2 Diagram showing the model components and inputs for Task 1. The radiative transfer model will be used to generate synthetic radiances, which will be analyzed by the observing system models. This task focuses on spectra of the Earth and other planets in this solar system because aspects of the thermal structure, composition, and optical properties of the planet's environment must be specified from observations.

The Earth's atmosphere and surface have been observed from a broad range of remote sensing instrumentation since the dawn of the space age. These data have placed important constraints on the Earth's thermal and solar radiation fields, but are not directly applicable to studies of the detectability of biosignatures in the atmospheres of extrasolar planets because (1) the spatially-resolved, LEO viewing geometry is substantially different than that for disk-integrated observations of distant worlds, and (2) these observations cover only a fraction of the solar and thermal spectra.

The models and methods described below will be used to explore the following questions concerning the detection of astronomical biosignatures from extrasolar planets:

- What does the spectrum of Earth look like from the UV to the far-IR (beyond the range of current Earth-based satellite data)?
- What information on atmospheric physical parameters and chemical composition can we derive from these spectra, and at what spectral resolution and signal to noise do we start losing this information?
- What is the spectral signature of biogenic processes in the Earth's atmosphere?
- At which wavelengths are biosignatures most easily detected?
- Can these spectral signatures be detected and discriminated in observations by existing or planned terrestrial planet detecting instruments?
- How does the presence of clouds and aerosols affect the detectability of biosignatures in the Earth's atmosphere and the optimum spectral regions for detection?
- What spectral resolution do we require to distinguish between possible sources for the biosignature molecules, and to determine the level of disequilibria?
- Can we distinguish the difference between an atmosphere with a boundary layer of rock, or a boundary layer of vegetation (chlorophyll)?
- What common spectral features in abiotic planetary atmospheres (Venus, Mars) can mask or masquerade as biosignatures (false positives)?
- To what extent does the spatial integration over the disk of the planet reduce the detectability of physical, chemical, and biological information in its spectrum?
- How do these disk-averaged spectral signatures change with observing geometry (day/night, pole/equator) or season?

Even though the available observational data is not adequate to directly address these questions, it is more than adequate to constrain atmosphere-surface radiative transfer models of this system. Here, we propose to use a comprehensive suite of radiative transfer models, and the best available constraints on the terrestrial environment, to produce synthetic spectra of the Earth's atmosphere over the largest possibly wavelength range. These results will be analyzed with the aid of sophisticated instrument models that can simulate the sensitivity of the current planned instruments to be used for detection and characterization of extrasolar planets. These models and their inputs are described in the following section.

C.3.1.2 MODELS

The Radiative Transfer Models

A comprehensive suite of atmospheric radiative transfer algorithms have been developed as part of our ongoing NASA Planetary Atmospheres and Planetary Astronomy tasks. These models have been extensively tested in applications with atmospheric compositions and temperature structures as diverse as the deep atmosphere of Venus (Meadows and Crisp, 1996), the atmospheres of the Earth (Crisp 1997) and Mars (Bell et al. 1993), and the upper atmosphere of Neptune (Crisp, 1995). They have also been used for studying cometary atmospheres (Brooke et al. 1996) and for determining the effects of the impacts of Comet Shoemaker-Levy 9 with Jupiter (Meadows et al. 2000). The radiative transfer models and supporting programs are described in detail below.

SMART

The Spectral Mapping Atmospheric Radiative Transfer (SMART) model, is the principal model that will be used to generate the high-resolution synthetic spectra of planetary atmospheres for this task, and for all the subsequent tasks. It will also be used to generate solar and thermal radiative fluxes and heating rates for the climate and chemistry modeling calculations proposed in Tasks 2-4.

SMART is a multi-stream, multi-level, spectrum-resolving (line-by-line) multiple-scattering algorithm. Using a high-resolution spectral grid it completely resolves the wavelength dependence of all atmospheric constituents, including absorbing gases (infrared absorption bands, UV pre-dissociation bands, and electronic bands) and airborne particles (clouds, aerosols) at all levels of the atmosphere, as well as the wavelength-dependent albedo of the planet's surface, and the spectrum of the incident stellar source. In addition, SMART employs innovative high-resolution spectral mapping methods (c.f. Crisp and West, 1992; Meadows and Crisp, 1996; Crisp 1997) to minimize the number of monochromatic multiple scattering calculations needed to generate high resolution synthetic spectra for broad spectral regions (c.f. Figures C.1.2 and C.3.1).

SMART generates a high-resolution, angle-dependent radiance spectrum through the following series of steps. It first defines the composite (gas and particulate) optical depths, single scattering albedos and scattering phase functions for each atmospheric layer, at each spectral grid point, in a multi-layer, scattering, absorbing atmosphere. Surface albedos and bi-directional reflection functions are also specified as the lower boundary of the model, and solar (stellar) fluxes are determined at the top of the atmosphere at each spectral grid point. Next, the spectral mapping algorithm employs a user-defined binning criteria to identify all spectral grid points that have optical properties that remain similar at all levels of the atmosphere and at the surface (c.f. West et al. 1990). Similar monochromatic intervals are collected into bins. SMART records the bin number associated with each spectral grid point to create a spectral map. SMART then uses the multi-level, multi-stream discrete ordinate algorithm, DISORT (Stamnes et al. 1988), to compute the angle-dependent radiances for each spectral bin. Finally, it uses the spectral map to distribute these radiances back into their original spectral positions to create a high-resolution radiance spectrum. The results of this model for remote-sensing observations have been tested and shown to be highly accurate, because it uses all of the available information about the atmospheric and surface optical properties, and employs a minimum number of approximations.

The innovative spectral mapping algorithm allows high accuracy with enhanced computational efficiency. In broad-band radiance and heating rate calculations for the atmospheres of Venus, Earth, and Mars, a direct, line-by-line calculation requires about 10^7 monochromatic spectral grid points to resolve the solar and thermal spectra. When compared to a brute force line-by-line model with the same capabilities, SMART usually requires only about 1% as many monochromatic multiple scattering calculations to completely resolve the wavelength dependence of the surface and atmospheric optical properties. The radiance fields generated by this model rarely differ from those produced by the full- line-by-line models by more than 1 to 2% in spectral regions wider than 1 cm^{-1}. SMART therefore provides both the speed and accuracy needed for all of the radiative modeling applications envisioned for this program. Examples of SMART spectra for Venus, Earth and Mars are shown in Figures C.3.1.

In summary, SMART provides the following improvements over the existing models used to study biosignature detectability:

- simulates both solar/stellar and thermal sources,
- includes a rigorous (monochromatic) treatment of multiple scattering by gases, clouds, and aerosols, at both solar and thermal wavelengths (Figure C.1.2),
- can use all available constraints on the wavelength-dependent optical properties of gases, airborne particles, and a reflecting surface,
- can incorporate all available constraints on the vertical distributions of temperatures, trace gases, and airborne particles (clouds, aerosols),
- provides a detailed, angle-dependent description of the radiation field, facilitating the derivation of disk-integrated results from any viewing angle,
- evaluates spectrally-integrated fluxes throughout the atmosphere, facilitating the derivation of solar heating rates, thermal cooling rates and photochemical reaction rates.

The Line-By-Line Model For Gas Absorption, LBLABC:

A spectrum resolving (line-by-line) radiative transfer model like SMART require a comprehensive, wavelength-dependent description of the absorption by gases. To address these needs, we developed the state of the art line-by-line model, LBLABC. Unlike the line-by-line algorithms used by the terrestrial radiative transfer modeling community, LBLABC was designed to compute the absorption by rotational, vibration-rotation, and pre-dissociation lines over a very broad range of pressures (10^{-5} to 100 Bars), temperatures (130 to 750 K), and line-center distances (10^{-3} to 10^{3} cm^{-1}). LBLABC completely resolves these features at each level by evaluating the gas absorption coefficients on a series of nested spectral grids. This multi-grid approach requires only 100 to 200 evaluations of the line-shape function for each spectral line, even when very high resolutions are needed (10^{-3} cm^{-1}) and lines contribute significant absorption at distances as large as 1000 cm^{-1} from the line center (as they do in the deep atmosphere of Venus). Once the absorption coefficients have been obtained for all lines that contribute to the spectral interval of interest, contributions from each grid are interpolated to a single high-resolution output grid, summed, and then saved to disk.

To accurately simulate the absorption throughout a planetary atmosphere, LBLABC employs a different line shape function in the line-center, near-wing, and far-wing regions of spectral lines. For line-center distances less than 40 Doppler halfwidths, a Rautian line shape is used. Like the commonly-used Voigt line shape, the Rautian line shape incorporates Doppler broadening and collisional (Lorentzian) broadening, but it also includes collisional (Dicke) narrowing, which can be important for lighter molecules. At greater line-center distances, LBLABC uses a van Vleck-Weisskopf profile for all gases except for H_2O, CO_2, and CO (c.f. Goody and Yung, 1989). The super Lorentzian behavior of the far wings of H_2O lines is parameterized by multiplying the Van Vleck-Weisskopf profile by a quasi-empirical, wavenumber-dependent χ factor. The χ factor recommended by Clough et al. (1989) has been adopted in most of our published work, but a new ab-initio far-wing line shape formulation recently developed by Ma and Tipping (1992) will also be tested for the simulations proposed here. These profiles provide significant absorption at line-center distances exceeding several hundred wavenumbers. This absorption accounts for the water vapor continuum absorption seen at thermal infrared wavelengths, and even produces a weak continuum throughout much of the visible and near-infrared spectrum (Crisp 1997).

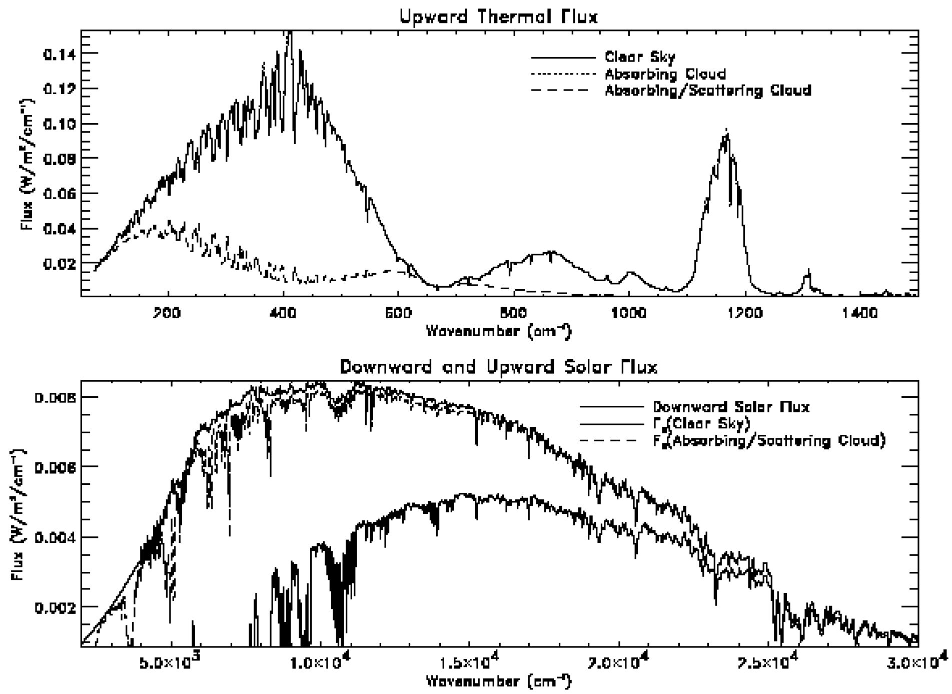


Figure C3.3 The effects of neglecting scattering when modeling CO_2 clouds. Top: The upward thermal flux emitted by a 5-bar CO_2/H_2O/CO atmosphere for a clear sky case and for cases with CO_2 clouds that absorb only, and absorb and scatter. When scattering is neglected, the clouds have very little effect on the upward thermal flux at the top of the atmosphere. However, the more realistic absorbing and scattering cloud produces a significant reduction in the upward thermal flux over both the clear sky and absorbing cloud cases. Bottom: A comparison of the upward solar fluxes for the clear sky (narrow solid line), and CO_2 cloud (dashed line) cases, shown here relative to the incident downward solar flux (thick solid line). Compared to the clear sky case, CO_2 clouds reflect back the vast majority of the incident flux, thereby increasing the planetary albedo. Realistic modeling of planets with CO_2 clouds cannot be achieved with models which neglect the effects of scattering.

The CO_2 line profile can be more accurately simulated by assuming a sub-Lorentzian line shape (Burch et al. 1969). Recent theoretical work (c.f. Levy, 1992) has now confirmed that this behavior is primarily a consequence of a vibration-rotation energy redistribution process called *collisional line mixing*. LBLABC includes an explicit physical line mixing algorithm for CO_2 Q-branches, where these effects are most pronounced (Hartmann and Boulet, 1991), and a semi-empirical technique is needed for CO_2 P- and R-branches (c.f. Meadows and Crisp 1996). These methods should provide the accuracy needed for the calculations proposed here, but more rigorous methods are continuously being sought to support our ongoing planetary atmosphere modeling tasks.

Single Scattering Optical Properties Of Cloud And Aerosol Particles:

To provide an accurate description of the solar and thermal radiation fields in cloudy or aerosol laden atmospheres, spectrum-resolving multiple scattering models like SMART require a detailed, wavelength dependent description of the single scattering optical properties of the cloud and aerosol particles. This information is essential both for the retrieval of cloud and aerosol properties from remote sensing observations, and to estimate their contributions to the solar and thermal radiative forcing in climate models. For the simulations proposed here, we will use our existing suite of single scattering particle codes. These include Mie scattering models for spherical particles (Wiscombe, 1980), T-matrix models for axisymmetric non-spherical partiles (Mishchenko, 1991), and Geometric Optics/Modified-Kirchhoff models for large ice crystals (Muinonen et al. 1989). This suite of models can produce an accurate description of the particle optical properties over the broad range of sizes, shapes, and wavelengths needed in this investigation.

C.3.1.3 MODEL INPUT

In addition to the planet-specific input parameters, such as the horizontal and vertical distributions of surface and atmospheric temperature, trace gas concentration, clouds and aerosols, and surface cover, the radiative transfer models require a number of laboratory data sets. These include:

- molecular line databases needed to generate the line-by-line description of infrared vibration-rotation bands of gases,
- UV and visible cross-sections of gases associated with electronic and pre-dissociation transitions in gases (e.g. ozone)
- the wavelength-dependent dielectric properties of photochemical aerosols and condensate cloud droplets needed to generate their single scattering properties.

The last two of these databases have been compiled over the years for simulations of the Earth and other planets in our solar system, and should be adequate for the work proposed here. We also have compiled extensive molecular line databases, but these must be augmented for the proposed modeling tasks.

Molecular Line-list Databases

Comprehensive, up-to-date molecular line lists are needed to provide the most complete wavelength coverage for molecular spectral features. This information is important to ensure that we miss as few spectral features attributable to an atmospheric constituent as possible. Less complete line lists may cause us to fail to identify a potential biosignature or to make a mistake in assessing the detectability of a biosignature. Although much work has been done on line lists for many of the common bulk atmospheric constituents, potential biogenic molecules, e.g. OCS, SO_2, CH_3SCH_3 (dimethyl sulfide) and S_8, will be specifically targeted for extra study in this project.

Complete wavelength coverage throughout the infrared is also advantageous because it allows us to correctly model the radiative balance in a planetary atmosphere for bulk constituents that are strong absorbers. Also, for the work proposed in this task, it allows us to generate *predictive* synthetic planetary spectra for wavelength regions for which we have no observational data.

C.3.1.4 WHAT IS A LINE LIST?

Line lists are compilations of molecular parameters for spectral lines that allow us to recreate line intensities, shapes and positions with line-by-line models, such as LBLABC. Line list parameters include the wavelength of the line center, lower state transition energies, transition line intensities, and line shape parameters as a function of temperature. Typically, many tens of thousands of ro-vibrational transitions contribute to the spectral signature of a particular molecule.

Table C.3.1: Summary of available molecular line-list databases

DATABASE$^+$ and WEBSITES	region$^\#$ cm^{-1}	number of species	millions of transitions	Ref.
1996 JPL catalog http://spec.jpl.nasa.gov	0 - 330 -	331 "entries"	1.5	14
1997 SAO-rotational http://firs-www.harvard.edu/dir/sao92	10 - 1600	49	0.5	16
1997 GEISA http://ara01.polytechnique.fr	0 - 22,600	50	0.7	13
1996 HITRAN http://CFA-www.Harvard.edu/HITRAN	0 - 22,600 - 58,500	46	1.0	11
1996 HITEMP	0 - 23,000?	3 or 4 ?	2.3	12
1995 ATMOS	0 - 10,000	49	0.8	15
1996 JPL VUV Reference Data http://remus.jpl.nasa.gov/jpl97	Vis-UV	≈ 65	cross sections	7
1993 Hanst Digitized IR Spectra	500 - 4000	250	lab spectra	17

The most widely used collection of molecular parameters available in electronic form is the HITRAN (High resolution Transmission) database (Rothman et al. 1998). However, there are a number of other spectroscopic databases available, as summarized in Table C.3.1 The HITRAN database is updated every two to five years using data collected in new laboratory studies. To obtain the information required to create line lists for new molecules or new regions of the spectrum, one or two spectra of different optical densities are recorded with a high-resolution spectrometer. The quantum numbers of the observed features are then identified (quantum assignments), and theoretical quantum mechanical models are manipulated in an attempt to reproduce the energy levels. If the modeling is successful, a reliable prediction of positions, lower state energies and relative intensities can be made for the molecular databases. However, the absolute intensities are still required before the predictions can be used for atmospheric measurement and modeling. These intensities and widths are usually measured using least squares curve-fitting techniques (Brown et al. 1983) and analyzed as separate efforts that involve from 5 to 50 spectra. Thus the information needed for a good compilation usually comes from several different studies. Therefore a key step in forming a more-comprehensive compilation for a given molecule is collating the available lab data and merging relevant sources. For heavy molecules like the freons or organic molecules with more than six atoms, the spectra are unresolved bundles of transitions that are not readily characterized through a line-by-line approach. To provide some limited information about the molecular absorption features, laboratory spectra are analyzed to yield wavelength-dependent absorption cross-sections. The Hanst and Hanst catalog (Table C.3.1) is a commercially available collection of low resolution laboratory data which provides these approximate cross sections. Figure C.3.4 shows a low resolution spectrum of dimethyl sulfide from this catalog. Better parameters for some heavier species can also be obtained using a collection of high-resolution spectra recorded to support the ATMOS experiment (Brown et al. 1987).

In the type of planetary modeling envisioned here, it is also important that we obtain line lists for a wide range of temperature regimes, and in particular that we understand the so-called "hot bands" in atmospheres that are near the limits of the habitable zone. We already have extensive experience modeling the remotely sensed atmosphere of Venus, and spectra of the several hundred to several thousand degrees Kelvin impacts of Comet SL-9 with Jupiter. For these tasks, we have collated HITEMP databases for CO_2 (Wattson and Rothman, 1992) and H_2O (Paltridge and Schwenke, 1997), and also have high temperature line databases for CH4 (c.f. Hilico et al., 1994) and NH_3.

During the course of the modeling work the science team will identify important species whose molecular parameters are too poorly characterized to generate reliable extrasolar planet spectra, or will require molecular parameters for temperature regimes not currently supported. If no information exists for these species, we will record new laboratory spectra using the McMath Pierce Fourier transform spectrometer. This instrument is maintained by the National Solar Observatory at Kitt Peak National Observatory near Tucson, Arizona and is described in more detail in the facilities section. In summary, as input to the radiative transfer model, we will obtain the best possible spectroscopic databases for all important species, and create customized databases where necessary. Most of the information will be taken from existing databases (Table 1) and reported laboratory studies in the literature, but we will acquire new data, where necessary, using the McMath FTS. The objective of this activity will be to obtain a database of molecular parameters that is as complete as possible with intensities accurate to 25% or better

Planetary Insolation-The Spectrum of the Parent Star

For Task 1, we will model only planets within our own solar system. For these simulations, we will use a high-spectral-resolution solar spectrum compiled from satellite observations at UV wavelengths (Atlas-2 SUSIM) and stellar atmosphere models at longer wavelengths (Kurucz, 1995). In Task 3 and beyond, high-resolution spectra of other stellar types will be used.

Astronomical Instrument Simulators

The generation of synthetic spectra of planetary atmospheres with the radiative transfer models is the first step in determining the detectability of biosignatures by astronomical instrumentation. The next step is to input these spectra into a model simulator that can explore the detectability of these biosignatures as functions of telescope and instrument design and the stellar environment surrounding the extrasolar planet.

Click to see figure C.3.4. Click on the figure to return back to here.

Figure C.3.4 Example of a simulated TPF spectrum of a Earth-like planet at 10 pc. The black body spectrum (no atmosphere) is indicated by the solid line. The symbols (filled triangle and diamond) represent the fluxes measured at each wavelength from the simulated TPF images. The simulated data corresponds to a dual 3-element nulling interferometer and 20 days of integration. Note that the atmospheric features are clearly visible in the simulated spectrum

To this end, we will modify an existing model which is being used to produce S/N estimates for a range of instrument configurations and designs for first generation telescopes and instruments such as Terrestrial Planet Finder (TPF). TPF is currently based on a nulling-interferometric design, and is optimized for observing in the mid-infrared, where the parent star is "only" a million times brighter than an orbiting terrestrial planet (rather than a billion times brighter as is the case at optical wavelengths). However, we will explore the detectability of biosignatures not only at the mid-infrared wavelengths available to the nulling interferometers (Figure C.3.4), but also in the near-infrared and optical, where extrasolar planet detection may be achievable using coronagraphic instrumentation.

Simulations for Nulling Interferometers

Recent simulations suggest that nulling interferometers operating in a 1AU orbit with four 3.5-m telescopes can detect Earth-like planets at distances as far as 15 pc and characterize their atmospheric emission for biosignatures. A smaller system using ~2.5-m apertures could still detect Earth-like planets but would not be able to search for the molecular gaseous absorption features that may be signs of life, such as ozone, in any but the nearest planetary systems.

These first generation instruments could be implemented in wide variety of configurations, constrained by the number of telescopes, the necessary degree of starlight and background suppression, and the required accuracy of the reconstructed images. There is a performance trade-off between combining many telescopes into a single array, to provide a deep and wide null to suppress starlight, and the ability to chop rapidly and to suppress large-scale diffuse emission from a zodiacal cloud by chopping between sub-arrays with relatively shallow nulls (Velusamy, Shao and Beichman, 1999). TPF may be designed with the ability to optimize its performance on-orbit using a number of separate beam-combiner modules which will allow chopping to be selected as needed. Many different instrument configurations are possible, and some of the key essential astronomical and instrumental factors affecting the ability of TPF to meet its goals include

- The size, temperature, and atmospheric composition of the target planet.
- The distance to the stellar system
- The luminosity and physical size of the star
- The distribution and amount of material of the zodiacal dust in the target system.
- The inclination of the orbital plane to the line of sight.
- Observatory properties such as the size and temperature of the telescopes and associated optics, interferometer baseline and nulling configuration, pointing jitter, etc.
- Instrument properties such as optical efficiency, detector dark current, depth and stability of the null.
- Local background due to dust in the solar system at the observing location and in the direction of the target.

Each of these factors will be included in the instrument simulator models to best determine the detectability of identified biosignatures using these first generation designs.

Simulations for Coronagraphs.

In addition to determining detectability for nulling interferometer designs, we will also explore the detectability of biosignatures for coronagraphic instrumentation. Coronagraphic architecture could provide direct imaging access, hence direct photometric and spectroscopic access to terrestrial planets orbiting nearby stars to distances of 10 pc and more. Depending on the wavelength range selected for the observations, the essential contrast requirements for a planetary companion may range from 10^{-6} to 10^{-10} times the star's peak intensity within a few tenths of an arcescond from the star.

The proposed investigation will be supported by computer simulations of coronagraphic telescope performance, based on computational tools developed for a number of recent JPL instrument concept studies. We will take advantage of an optical modeling capability developed to combine experience to date from space and the laboratory, with new optical designs for future space telescopes. These include a coronagraphic mode for the NGST near-infrared (1-5 microns) camera, a single filled-aperture telescope for TPF (1-15 microns wavelength), and a Discovery-class coronagraphic telescope of modest aperture working in the visible wavelength range (0.5-1.0 microns).

The simulation software developed for these studies is configured for a wide range of instrument designs. The telescope's architecture

- may include monolithic or multi-segment primary mirrors of arbitrary shape,
- can be configured with wide range of active wavefront correction technologies and their corresponding correction accuracies,
- may exhibit a range of mirror surface figure and polish characteristics scaled from a database of existing telescope surface characteristics, and
- includes a detailed simulation of wavefront phase retrieval from star images for alignment of active optics as implemented for NGST.

The sources of scattered light within the first few arcseconds of an isolated star image are well understood as a combination of diffraction from the pupil-defining obscurations, scatter from shallow mid-frequency surface figure errors (essentially the residual polishing marks on the 4- 40 cm scale), and stray scattered light traceable to inadequate baffling and dust in the optical path. In broad terms, these three sources are controlled by three technologies, respectively (1) a coronagraphic camera to reduce diffracted light, (2) telescope design and high-order active optical correction to reduce mid-spatial-frequency scatter, and (3) careful baffling and contamination control to mitigate unwanted stray light.

The software further includes the essential sources of background noise. The effects of optical scattering and diffraction in the telescope are combined with Zodiacal and exo-zodiacal light to estimate the background level against which a planet must be detected. Shot noise on this background and detector noise are included. The effective background noise from optical instabilities, including pointing jitter, focus drift, and thermal drift of the optical alignment, can be included to identify the outstanding specifications for optical system stability.

With these tools, we will be able to determine the sensitivity of coronagraphic observing instruments to biosignatures over the wavelengths covered by the study. We will also evaluate a number of feasible telescope configurations, and will provide recommendations for telescope design options and specifications required for biosignature detection.

C.3.5 INCREASES IN COMPUTATIONAL EFFICIENCY

The radiative-transfer modeling tools to be used for this task are computationally intensive. Therefore, increasing the computational throughput is essential to achieve our modeling goals. This will also be true of most of the models to be used in the subsequent tasks. In the course of this project we expect to generate several thousand simulations.

Currently the synthetic spectrum generating code, SMART, when modeling realistic, absorbing, scattering planetary atmosphere from only 1 to 2.5 microns takes about 3 hours running on a modern desktop workstation. Dramatic increases in computational efficiency can be obtained by moving to an appropriate parallel architecture. We therefore propose to implement these algorithms on two systems available in our

Ultracomputing Technology Research Group at JPL.

The first is a dedicated, 32-node BEOWULF parallel machine where each node is a Pentium II. This low-cost, dedicated machine is well suited for Data Parallel type of computation, that is, for computation with a very large degree of coarse grain parallelism and minimal inter-processor communication.

The second machine is a highly parallel Multi-Instruction-Multi-Data (MIMD) machine. This is a SGI Origin 2000 machine with 128 processor nodes. It is suitable for large-scale parallel computation and it is much more efficient for communication-intensive parallel computation.

For both machines, the approach is to first identify the computation-intensive kernels in the existing FORTRAN code and try to parallelize and optimize these kernels first. However, for a better result, and depending on the application, a more detailed algorithmic analysis might be needed and novel parallel algorithms may need to be developed. The central task for the first year of the proposed project will be an initial analysis of the existing FORTRAN code to choose the optimal hardware and software configuration for each simulation module.

C.3.1.6 RESEARCH APPLICATIONS OF THESE TOOLS

The first step in Task 1 is to analyze and upgrade SMART and LBLABC to increase their computational efficiency. With these upgraded radiative transfer tools, we will run a global grid of individual SMART simulations as a function of latitude, longitude and underlying surface. These simulations will generate angle-dependent radiance spectra extending from the UV through to the far-infrared. . These spectra will then be averaged over the planet's disk to produce a disk-averaged view that will simulate that available to astronomical instrumentation that does not explicitly spatially resolve the extrasolar planet.

To validate the accuracy of SMART over large wavelength ranges, the synthetic spectra will be averaged over the appropriate fields of view and compared to the available results from Earth-observing satellites (e.g. NIMBUS 4 IRIS, ADEOS IMG; ERS GOME, Galileo NIMS, and hopefully EO1 Hyperion).This validated technique will then be used to produce disk-averaged Earth spectra over a continuous wavelength range from the UV to the far-IR for changes in the following parameters:

- seasonal changes in trace gas distribution (solstices and equinoxes)
- changes in surface albedo for visible hemispheres dominated by land, ocean or snow/ice
- a range of cloud distributions from fully clear to fully cloudy
- a range of viewing phase angles (fractional illumination of the visible hemisphere).
- a range of viewing geometries (sub-Earth points) from equator-on to pole-on views.

These spectra will be used to determine astronomical sensitivity to variations in these parameters. The spectral resolution will be successively degraded to determine at which point we lose sensitivity. These spectra will then be processed with the astronomical instrument simulators to determine the sensitivity of these specific first generation designs to variations in these parameters.

We will then use this set of high-resolution spectra to identify potential biosignatures from the atmosphere and surface. We will then successively degrade the spectrum to note at which spectral resolution these features can no-longer be detected. We will also look for the detectability of seasonal variations in biosignatures. Finally, to identify possible false positive signatures, we run validation comparisons of synthetic spectra for Venus, Mars, and Titan, using the best available globally averaged data for these objects.

C.3.1.7 PRODUCTS AND SIGNIFICANCE FOR TASK 1

The primary products of the first task in this investigation include:

- The conversion of the radiative transfer models, SMART and LBLABC, for use on JPL's ultracomputing facilities. This is not only important for timely execution of this Task, it is the first step towards creation of the Fully-Coupled Virtual Planetary Laboratory.
- These models will be used to generate high-resolution, spatially resolved, spectra of Venus, Earth, Mars, and Titan that extend from the UV to the far IR.
- These spectra to will be studied to determine the effects of spatial and spectral averaging on the detectability of biosignatures and other spectral features that provide important

constraints on a planet's physical and chemical state and habitability.

These spectra will also be processed with observing system models for nulling interferometers and coronographs to determine how well the space-based instrumentation can detect and characterize extrasolar Earth-like planets, and discriminate them from abiotic planets (e.g. Venus and Mars). These results will be used to provide recommendations for the minimum and optimum spectral resolution, wavelength range, and signal to noise required for determination of atmospheric and surface physical and chemical parameters, for a range of terrestrial planets, and the detection of biosignatures in an Earth-like planet.

C.3.2 Task Two: The Spectral Signature of Thermodynamically Balanced Terrestrial Planets.

As the next step in the development of the Virtual Planetary Laboratory, we propose to implement a simple climate model to simulate the surface temperatures and atmospheric temperature profiles of extrasolar planets (Figure C.3.5). This is a logical next step because the thermal structure plays a dominant role in the infrared spectrum emitted by the planet. If the atmosphere includes condensable species, such as water, the atmospheric thermal structure will also control the distribution of clouds, which will affect the solar/stellar flux reflected by the planet and the vertical extent of the atmosphere that can be observed. Finally, the atmospheric thermal structure can affect the distribution of reactive trace gases of biological and abiotic origin through its effects on chemical reaction rates.

A variety of tools exist for determining the temperature distribution in terrestrial planetary environments. These tools fall into three major categories:

- 1D Energy Balance (1D EB) climate models (North et al. 1981),
- 1D radiative convective equilibrium (RCE) models (c.f. Manabe and Wetherald, 1967; Gierasch and Goody, 1968; Pollock et al. 1980; Crisp and Titov, 1997), and
- 3D General Circulation Models (GCM's).

The classical, diffusive, energy balance climate models provide a one-dimensional description of the pole-to-equator temperature distribution. These models have been widely used for studies of the effects of albedo on the energy balance, but they provide no direct constraints on the vertical distribution of atmospheric temperature or composition, or the details of the emitted spectrum.

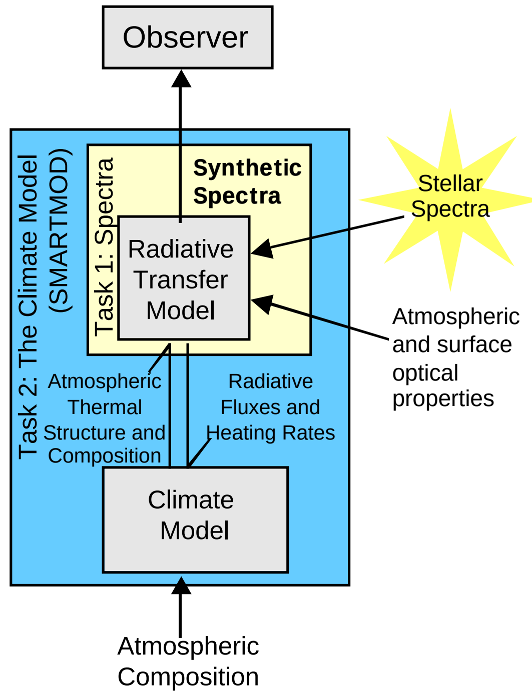


Figure C.3.5 Components of the Virtual Planetary Laboratory included in Task 2 are shown. The radiative transfer models are integrated with a climate model to produce a surface and atmospheric temperature distribution (and emitted spectrum) that is in thermal equilibrium with the specified atmospheric composition.

In contrast, 1D RCE climate models describe the globally averaged equilibrium temperature distribution with altitude in a planetary atmosphere with a given composition and incident solar flux. However, these models provide no direct constraints on the horizontal (equator to pole or sub-solar to anti-solar) temperature distribution. These horizontal variations can introduce changes in disk-integrated spectra of a planet viewed from different directions. For example, assume that the spectrum associated with the globally averaged RCE thermal profile is an excellent match to the disk-averaged spectrum of an extrasolar planet viewed from a point over mid latitudes (this works amazingly well for Earth). This spectrum will probably provide a much less satisfactory fit to the spectrum of the same planet viewed from other angles (ie. a polar view). Furthermore, the single global average spectrum may not adequately simulate the results of the spatial convolution of spectra from different parts of the planet. These arguments suggest that some estimate of the horizontal temperature variations is needed for studies of biosignatures on extrasolar planets.

In principle, a 3D General Circulation Model can provide constraints on both the horizontal and vertical distributions of temperatures in a planetary atmosphere. However, these models are much more complex and computationally intensive than the simple 1D climate models described above. Also, as we noted in the introduction to the task section, the reliability of these models depends crucially on the validity of a wide range of variables that will not be known for extrasolar planets for several decades. These parameters include the planetary rotation rate, axial obliquity, surface friction, topography, surface albedo distribution (ocean/land/ice), and many others. In addition, because these models must evaluate a host of parameters at thousands of horizontal grid points at every time step, they typically use relatively simple approximations for radiative forcing, convection, and other sub-grid-scale processes. These parameterizations can be tuned to yield good results for systems that are well constrained by observations, but they produce much less reliable results when applied to arbitrary environments. These factors, combined with the computational requirements of these models, suggest that, at this time, 3-D GCM's provide little real benefit to the study of extrasolar planetary environments.

For this investigation, we propose to use an efficient, hybrid climate model that incorporates advanced 1-D RCE and 1-D EB models to derive estimates of the temperature distributions in extrasolar planetary environments. A state-of-the-art 1-D RCE model will be used to derive solar radiative heating rates, thermal radiative cooling rates, and vertical convective heat fluxes for selected latitudes and solar longitudes. An EB climate model employing baroclinic adjustment (c.f. Stone 1978; Stone and Nemet, 1996) will then be used to estimate the exchange heat between these soundings. This approach has been widely used for studies of the Earth's present climate, terrestrial paleoclimates, and the atmospheres of other planets.

These methods are described in greater detail below.

C.3.2.1 MODELS

The Radiative-Convective Equilibrium Model

We are currently in the process of incorporating the Spectral Mapping Atmospheric Radiative Transfer (SMART) model (Task 1) into an existing 1D RCE, model, called RTMOD (Crisp 1989), as part of Meadows' ongoing NASA Exobiology task for modeling the effect of clouds on planets at the limits of the habitable zone. The combined RCE model, SMARTMOD, is currently undergoing testing and will be ready for routine use in this task by February of 2001.

SMARTMOD employs a number of innovative features that enhance its versatility and accuracy. First, unlike most 3-D climate models, which use highly simplified radiative transfer schemes, SMARTMOD derives a detailed description of the solar and thermal radiation fields using the full SMART algorithm (Task 1). It then uses an explicit time-stepping scheme to solve the 1-D thermodynamic energy equation as an initial value problem to yield the radiative equilibrium temperature profile consistent with the atmospheric composition and solar forcing. This time-marching approach is ideal for this application because it can accommodate changes in the optical properties of the atmosphere. For example, it can explicitly include changes in gas mixing ratios, cloud formation and dissipation, and surface albedo variations (ice accumulation and melting) that might occur as the temperature profile evolves.

SMARTMOD also employs a more physically realistic treatment of vertical heat transport by free convection. Most existing RCE models (Manabe and Wetherald, 1967; Pollack et al. 1980; Crisp 1989) use a simple "convective adjustment" to simulate the effects of convective heat transport. In contrast, SMARTMOD uses an explicit mixing length formulation (c.f. Gierasch and Goody, 1968) for moist or dry convection. This approach permits temperature discontinuities between the surface and the lowest atmospheric layer, and produces much more realistic temperature profiles near the surface. It also provides estimates of the vertical eddy diffusion rates, for use in atmospheric chemical models.

In addition to globally averaged temperatures, SMARTMOD can generate high-resolution spectra of the resulting equilibrium atmosphere with output parameters identical to those produced by SMART. The SMARTMOD results can therefore be analyzed by the observation system modeling tools employed in Task 1.

The Energy Balance Climate Model

To simulate horizontal (equator to pole or sub-solar to anti-solar) heat transport by atmospheric dynamics, SMARTMOD, will be incorporated with a simple, energy balance (EB) climate model. In the integrated model, SMART algorithm will be used to find the instantaneous solar heating and thermal cooling rates at several locations on the planet at each time step. These soundings can include clear and cloudy conditions and a variety of surface albedos over a range of latitudes and solar longitudes. The simple EB model will then use linear diffusion (c.f. North et al. 1981) to distribute heat between the soundings, and modify the atmospheric thermal structure for the next time step. This process will be repeated until the system reaches equilibrium.

On moderate to rapidly rotating planets (e.g. Earth, Mars), the meridional (equator to pole) heat diffusion coefficients will be parameterized by Baroclinic Adjustment (c.f. Stone, 1978; Stone and Nemet, 1996). In this approach, the zonal mean meridional atmospheric temperature gradients are compared to the critical gradient for baroclinic stability at each time step. If it exceeds this gradient, the down-gradient heat diffusion coefficient is increased, and heat is more efficiently transported downgradient to stabilize the horizontal temperature contrast. For slowly rotating planets, like Venus (or Titan), or in very statically stable regions in the atmospheres of more rapid rotators (i.e. the Earth's stratosphere), an empirical horizontal diffusion coefficient will be specified, and validated by comparing simulations with available observations.

C.3.2.2 MODEL INPUTS

Like the radiative transfer model described in Task 1, the climate models described above require a comprehensive description of the incident stellar flux, atmospheric composition, surface properties (albedo, thermal inertia) and the distribution of absorbing gases and aerosols. They also need the comprehensive line lists developed in Task 1. However, they only need relatively crude initial estimates of the atmospheric and surface temperatures to initialize the thermal equilibrium calculations.

Computational Efficiency

As part of this task, we will adapt SMARTMOD to run on the ultracomputing facilities at JPL. This is extremely important for achieving our stated goals in a timely manner, while maintaining the rigorous physical treatment of gases and aerosols provided by the SMART algorithms embedded in SMARTMOD.

C.3.2.3 RESEARCH TASKS

SMARTMOD Validation

The 1D RCE component of SMARTMOD is currently being developed independently of this CAN using Meadows' NASA Exobiology funds. The preliminary integration of SMART to RTMOD was completed this August, and the full integration of the two programs is expected to be complete by February 2001. The RCE component of SMARTMOD will be validated by generating globally averaged RCE temperature profiles for Venus, Earth, Mars, and Titan, and comparing these results to existing observations. In addition, the high-resolution synthetic spectrum of the equilibrium atmosphere produced by SMARTMOD will be validated against globally, annually, averaged observations for Venus (Venera 15 Spectrometer), Earth (NIMBUS 4 IRIS) and Mars (Mars Global Surveyor TES) to determine how well these spectra preserve important spectral features.

In parallel with this effort, SMARTMOD will be integrated with the EB climate model to provide a spatially varying description of the surface and atmospheric temperature distribution. The combined model will then be implemented on the JPL ultracomputing facilities. This integration effort should be completed before the end of FY 2001.

To validate this combined model, spatially resolved radiative-convective-diffusive temperature distributions will be generated for Venus, Earth, and Mars. These temperature distributions will be compared to the available observations of these planets to refine the horizontal diffusion coefficients, and to identify simple mechanistic relationships between these coefficients and the planet's bulk parameters (e.g. rotation rate, atmospheric density, surface albedo and thermal inertia, etc.). Finally, because the fundamental objective of this project is to identify biosignatures in disk-integrated, planetary spectra, SMARTMOD's spatially resolved, high-resolution spectra for the simulated atmospheres of Venus, Earth, and Mars will be averaged over the planet's disk for the range of viewing conditions considered in Task 1. These results will then be compared to the disk-integrated spectra derived using observed atmospheric properties in Task 1, to determine how well the climate model can simulate disk-integrated atmospheric spectra. This validation effort should be completed before July 2002.

SIGNIFICANCE AND PRODUCTS FOR TASK 2

Upgrade of SMARTMOD to incorporate a RCE and EB model, and the implementation of these tools on JPL's ultracomputing facility is an essential step toward the development of the Virtual Planetary Laboratory. The validation effort will also provide a number of products that will be of value to NASA's Astrobiology Program. For example, these experiments will produce an important advance in our understanding of the Venus greenhouse mechanism. This is important for planets near the limits of the habitable zone since earlier models included much a much less sophisticated description of radiative processes (e.g. band models, neglect of scattering at thermal wavelengths, etc., c.f. Crisp and Titov, 1997). The comparison of viewing-angle-dependent, disk-averaged spectra of Venus, Earth, and Mars obtained from SMARTMOD, and those produced directly from observations (Task 1) will also show how well the environment of an extrasolar planet can be simulated with a simple, efficient climate model.

C.3.3 TASK THREE: THE SPECTRAL SIGNATURE OF CHEMICALLY AND THERMODYNAMICALLY BALANCED ATMOSPHERES OF EXTRASOLAR PLANETS

To increase the versatility of the Virtual Planetary Laboratory, Task Three incorporates the radiative transfer and climate modeling tools developed in the first two tasks with a comprehensive, atmospheric photochemical model (Figure C.3.6). The resulting climate-chemistry model will allow us to create a wide-range of plausible model extrasolar planet atmospheres that are radiatively, thermally, and chemically self-consistent. With this tool, we will:

- initiate a study of biosignatures in the Earth's early atmosphere
- explore the detectability of the currently accepted list of potential biosignatures in both oxidizing and reducing atmospheres, for a variety of stellar types
- provide recommendations for instrument parameters and capabilities required to detect these biosignatures.

To address these goals, we need a versatile, modular, atmospheric photochemical model that can reliably simulate a wide range of conditions in the atmospheres of terrestrial planets. The comprehensive, state-of-the-art Caltech/JPL photochemical model will be ideal for this application. The following two sections describe the background and implementation approach of the chemical model. We then summarize the types of input data sets needed, and propose a series of specific experiments that address the goals listed above.

C.3.3.1 BACKGROUND:

NASA has conducted a nearly complete reconnaisance of the Solar System, having acquired close-up observations of every planet, except Pluto, and many moons. From these spacecraft missions and from ground-based and earth-orbiting telescopes, a detailed catalog of the chemical composition has been developed for every significant atmosphere. Atmospheric photochemical models have been able to quantitatively reproduce the essential compositional measurements of these atmospheres (Yung and Demore, 1999). The stability of the primarily CO_2 atmosphere of Venus and of the ozone layer in the Earth's stratosphere are maintained by catalytic reaction cycles involving oxygen-, hydrogen-, and chlorine-containing radical (highly reactive) chemical species that exist in these atmospheres in trace amounts. The stability of the CO_2 atmosphere of Mars and of ozone in the terrestrial mesosphere are maintained similarly by reactions involving primarily oxygen- and hydrogen-containing radical species. Complex hydrocarbon species are formed in the molecular hydrogen-dominated atmospheres of Jupiter, Saturn, Uranus, and Neptune as a result of the photolytic decomposition of methane and secondary reactions following the photolytic decomposition of acetylene, a primary product of methane dissociation. The cold nitrogen-dominated atmospheres of Titan and Triton have both methane photochemistry and the chemistry of reactive nitrogen species that leads to the formation of nitrile compounds (containing carbon-nitrogen chemical bonds).

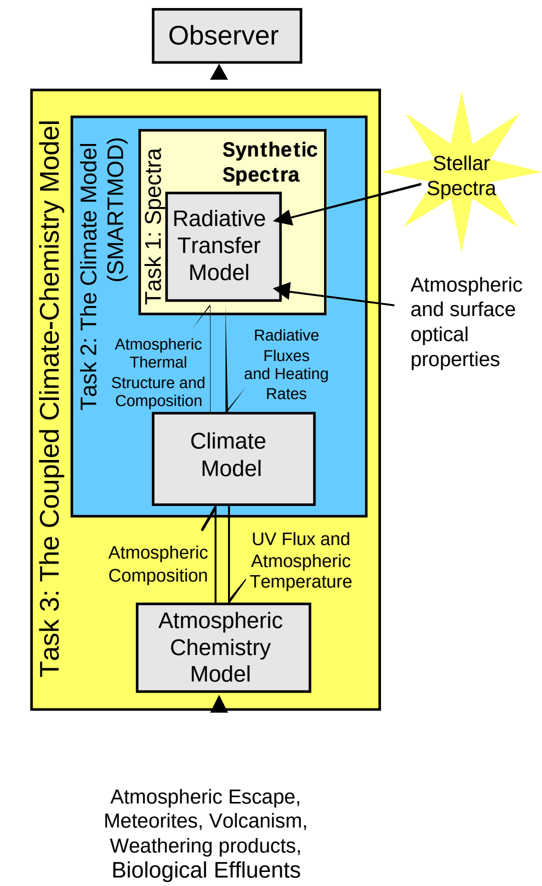


Figure C.3.6 Components of the Virtual Planetary Laboratory included in Task 3 are shown. The radiative and climate models are integrated with an atmospheric photochemical model to yield spectra of environments that are in radiative, thermal, and chemical equilibrium.

Yung and DeMore (1999) show that the chemical kinetics of the solar system can be reproduced with about two thousand reactions relating the interactions among several hundred species. One can point to the success achieved in explaining the observed composition of the primary atmospheres in the solar system as evidence of the success of this program. In addressing the question of the atmospheres of extrasolar planets, the planets of our Solar System can serve as a guide. The terrestrial and Jovian atmospheres represent the end members of oxidizing and reducing atmospheres, respectively. Titan is an intermediate case between Earth and Jupiter. In all cases a quantitative assessment is possible if the disequilibrium chemical forcing on the system can be quantified.

The Caltech/JPL planetary atmosphere model has been used to simulate and quantitatively reproduce modern observations: Venus (Yung and Demore, 1982; Mills, 1999), Earth stratosphere (Froidevaux et al., 1985; Allen and Delitsky, 1991), Earth mesosphere (Allen et al., 1981, 1984), Mars (Nair et al., 1994), Jupiter (Allen et al., 1992; Gladstone et al., 1996), Saturn (Moses et al., 2000a, b), Titan (Allen et al., 1980; Yung et al., 1984), Neptune (Moses et al., 1992), Triton (Lyons et al., 1992), and the Jovian planets (Lee et al. 2000).

C.3.3.2 MODELS

The 1D Chemical Model

The Caltech/JPL general planetary atmosphere model is a multidimensional model that simulates the chemical composition of a planetary atmosphere, accounting for the coupling of photochemistry and atmospheric transport. The modular design of the code provides great flexibility in simulating a wide variety of chemical environments. In addition to the atmospheric chemistry of the Earth and other major Solar System bodies, the model has been used to simulate cometary comae and interstellar molecular clouds.

The Caltech/JPL planetary atmosphere model includes a one-dimensional (1D) mode. In this mode, it produces a vertical distribution for each selected chemical constituent by solving the time-dependent (steady-state in the case of long timesteps) continuity equation consisting of terms for the local production and loss of the chemical species and vertical diffusive transport (Allen et al., 1981). Vertical transport includes eddy, molecular, and thermal diffusion (Banks and Kockarts, 1973). The complete, coupled set of continuity equations (one for each constituent) is solved simultaneously using a finite-difference iterative algorithm adopted from Richtmeyer (1957).

When this chemical model is used in isolation, the physical structure of the atmosphere is prescribed. Once coupled with the climate model, developed in Task 2, the physical structure can be self-consistently determined. Calculations are performed on a vertical grid with an arbitrary number of levels and at each level total atmospheric pressure, temperature, and eddy diffusion coefficient are defined. The physical structure can be updated during a chemical model run.

The model can handle an arbitrary number of chemical constituents interrelated by an arbitrary number of chemical reactions. Processes occurring above and below the boundaries of the modeled atmospheric column and processes occurring at these two spatial interfaces are parameterized by fixing the abundance of a constituent at a boundary or by selecting one of several formulations for mass flux into or out of each boundary. These boundary conditions also can be updated in the course of a model run.

C.3.3.3 MODEL INPUT

The photochemical model requires a library of kinetic reaction rates, as well as constraints on UV fluxes and the atmospheric thermal structure. It can also accommodate arbitrary sources or sinks at the upper and lower boundary. The chemical kinetic data needed for the experiments proposed here has been compiled over a number of years, and are readily available to the team (c.f. Demore et al. 1992). The atmospheric physical properties can be obtained from the coupled radiative and climate models.

However, the addition of a comprehensive atmospheric photochemistry model provides opportunities to initiate our investigation of the chemistry in the atmospheres of terrestrial planets around stars with spectral types that are different than that of the sun. Task 3 therefore includes a focus on obtaining realistic spectra of these stars. This input data is also needed to refine our understanding of the Habitable Zone and the detectability of biosignatures by using realistic stellar spectra as the radiation source at the top of extrasolar planetary atmospheres.

Stellar Spectra

Another critical input to radiative transfer, climate, and chemical models of terrestrial planet atmospheres is the wavelength-dependent radiative input from the parent star. Traditional calculations of stellar "habitable zones" (HZs) have represented the stellar emission spectrum as black bodies for all but the G2V case, where the Sun's spectrum was used (Kasting 1993). Over the past decade, there has been a major effort to establish accurate, detailed, absolute calibration stars in the infrared, spanning the 1-30 μm range, with extensions to 300 μm to support specific space-based instruments. This work graphically demonstrates that no star radiates as a blackbody and that stellar spectral energy distributions (SEDs) are invariably mutilated, even at low spectral resolution, by strong absorption bands. Planets have now been discovered around stars with spectral types ranging from F7 to M2V. Examples of the extreme departures of realistic stellar spectra from blackbodies over this spectral range can be seen in Figure C.3.7.

The use of black body approximations for spectra of stellar types other than our own Sun may be adequate to indicate crudely the scale of the HZ around a variety of stars (e.g. Cohen 1999, Kasting 1993). However, more realistic stellar spectra would improve our ability to assess the correct integrated luminosity incident on a planetary atmosphere. Improved estimates of the spectral distribution of the stellar energy incident on a planet would also improve the accuracy of both radiative balance calculations and photochemistry in planetary atmospheres. In addition, the spectrum of the parent star may affect the detectability of features in a planetary atmosphere. For example, many of the molecular signatures of the terrestrial atmosphere can be found as absorption features in the spectra of the host stars, e.g. H_2O, CO, CO_2. Consequently an effort to detect CO_2 (in the red wing of the CO fundamental) or O_3 (within the SiO fundamental) might become quite difficult, especially at low spectral resolution. These considerations suggest that state-of-the art representations of stellar radiation spectra are an essential part of a rigorous investigation of the detectability of astronomical biosignatures.

Click to see figure C.3.7. Click on the figure to return back to here.

Figure C.3.7 Comparisons between Kurucz and NextGen model spectra and photospheric blackbodies for F7V and M2V stars. The blackbodies are presented simply to show deviations of the shape of real stars from those of blackbodies. The blackbody has been normalized to one point on the entire UV-mid-IR spectrum for each spectral type, so the separate UV and mid-IR diagrams show consistent scaling. Large deviations from a blackbody can be seen for both spectral types, especially for the UV region of the stellar spectrum. The features near 2.3 and 4.7μm are CO 1st overtone and fundamental bands, but the dominant opacity from 5-8μm is water vapor, with a small contribution from the SiO fundamental.

There is now a network of about 450 absolute calibrators derived from observations whose low-resolution ($\lambda/\Delta\lambda$~100) absolute spectra have supported several recent satellites (Cohen et al. 1999 & references therein). A major legacy of the recent ESA International Space Observatory is a set of higher resolution ($\lambda/\Delta\lambda$~1500) stellar spectra emphasizing a range of stars in which molecules play a dominant role. There has also been a corresponding growth in the creation of model grids for a wide diversity of stars, with associated synthetic spectra with resolutions ($\lambda/\Delta\lambda$) in the range ~100-100,000. The primary resource for years has been the set of computations by Kurucz (1992), which cover stellar classes from B to early K-types. For later-type stars, his models have traditionally lacked strong IR bands whose presence in stellar spectra was unrecognized for many years. For example, the SiO fundamental has a prominent head near 7.5 μm but extends beyond 11 μm.

To synthesize meaningful spectra for cooler stars, NextGen grids of models (Hauschildt et al. 1999a,b) are preferred to the standard Kurucz models. NextGen includes many more sources of molecular opacity than does Kurucz. To explore spectra of cool stars, the NextGen models now incorporate 313 million lines of water vapor (Partridge & Schwenke 1997), 12 million TiO lines (Jorgensen 1994), and the best available line lists for relatively common molecules such as CO (Goorvitch & Chackerian 1994a,b) and SiO (Langhoff & Bausclicher 1993).

In the wake of the ISO mission, and in preparation for SIRTF, there is currently a major effort to compare and contrast synthetic and observed IR spectra, and to interpret the differences. Leveraging this work, we will use these improved stellar models to represent the stellar radiation fields used as input to the Virtual Planetary Laboratory. We will use the Kurucz models for warmer stars (above ≈4000K), and the NextGen models for cooler stars. All these models provide synthetic spectra extending from the far-UV through to the far-IR. However, we will also make an effort to absolutely calibrate ISO observed spectra for cool stars (now archived) at resolutions of ~1500 in the 2-12 μm region.

Although these observations cover a smaller range of stellar types than the model grids, this approach would provide more realistic spectra over this wavelength range, in comparison to models that rely on parameterized atmospheres and molecular line lists.

C.3.3.4 UPGRADING THE CHEMICAL MODEL TO ULTRACOMPUTING.

The computational efficiency of the Caltech/JPL model will be improved by re-coding certain portions of the model to take advantage of the capabilities of the JPL massively parallel-processing computers. The evaluation of the internal atmospheric radiation field at each wavelength is independent of the other wavelengths. Similarly the evaluation of the chemical production and loss terms at each atmospheric level is independent of the other levels. Both sets of computations occur many times during the course of a single model run. We therefore expect significant improvements in the performance of this model.

C.3.3.5 RESEARCH TASKS

This task includes 2 sub-tasks. The first focuses on simulations of the Earth's paleo environment. The second involves preliminary simulations of a range of extrasolar planets around stars with different stellar types.

Biosignatures of the Early Earth

The chemical history of Earth's atmosphere currently provides our only record of the evolution of an atmosphere that has been influenced by biology. Over the past several years considerable progress has been made in reconstructing the first half of this record (prior to 2 billion years ago) by: (1) tightening empirical constraints on oxygen (Rye and Holland, 1998), (2) establishing the first empirical constraints on CO_2 (Rye and Holland, 2000a; Rye et al., 1995) and (3) suggesting plausible constraints on methane levels (Rye and Holland, 2000b). This work points to an early Earth radically different from today's Earth and has helped drive the push to understand how microbially-active planets with oxygen-poor atmospheres might appear from space.

The geologic record is consistent with the notion that atmospheric oxygen levels were very low during the first half of Earth history and rose sharply sometime around 2 billion years ago (Ga) (for early insights into this history see: Cloud, 1968; Holland, 1958; Holland, 1962; Holland, 1984). The behavior of Fe during weathering of paleosols (ancient soils) that formed before 1.7 Ga indicates that atmospheric oxygen levels were ~ 3 x 10^{-4} atm before 2.3 Ga and 0.03 atm after 2.0 Ga (Rye and Holland, 1998). Several other compelling lines of evidence from the sedimentary record support these conclusions. The presence of detrital pyrite (Ramdohr 1958a,b; Rye and Holland, 1998 and references therein) as well as of detrital siderite (Rasmussen and Buick, 1999) in sedimentary rocks that formed before 2.3 Ga indicate that oxygen levels were very low prior to 2.3 Ga. The worldwide emergence of red beds around 2.2 Ga indicates oxygen levels were already fairly high about 2.2 Ga (Rye and Holland, 1998 and references therein). A prolonged excursion to strongly positive values in the marine $\delta^{13}C$ record indicates that a large amount of oxygen was added to the atmosphere between 2.22 and 2.06 Ga (Karhu and Holland, 1996). For an alternative view see Ohmoto (1996 and 1997) and Watanabe et al. (1997), in which Ohmoto and his colleagues have concluded that the sedimentary and paleosol record contains no evidence of a major change in atmospheric oxygen levels over the past 3 to 4 Ga. However, the preponderance of evidence, including evidence of the sorts cited by Ohmoto and colleagues in the references cited above, is consistent with the hypothesis that oxygen was low until about 2 Ga.

Rye et al. (1995) found that atmospheric CO_2 was ~0.02 bar between 2.75 and 2.2 Ga. Their conclusions were based on the observation that Fe and Mg were distributed in paleosols of that era in a manner consistent with the precipitation of Fe-rich smectites and inconsistent with the precipitation of more than trace amounts of Fe-carbonate, siderite. Rye and Holland (2000a) found that the distribution of Ni, Co and Mn in the circa 2.2 Ga Hekpoort paleosols also was consistent with the precipitation of Fe-smectite in the lower portions of early paleosols. Siderite would have been the dominant Fe-mineral if atmospheric CO_2 was > 0.02 bar.

One-dimensional climate models suggest that greenhouse forcing equivalent to CO_2 > 0.1 bar was necessary to compensate for the fainter sun at 2.75 Ga (Kasting, 1987 and 1998). Another greenhouse gas that might have made up for the deficiency in CO_2 is CH_4, which is primarily a biogenic gas on Earth. There is isotopic evidence for non-marine methanotrophy ca. 2.75 Ga in lacustrine sediments (Buick, 1992) and at the top of a paleosol (Rye and Holland, 2000b). These observations suggest that atmospheric CH_4 may have been >20 ppm at that time and that biogeochemical processes involved in both the production of methane (methanogeny) and the consumption of methane (methanotrophy) may have helped to regulate the redox state of Earth's atmosphere as well as Earth's climate.

As well as using the best available constraints on the Earth's paleoatmosphere derived from the geological record, we have also initiated a collaborative agreement to work closely with the Carnegie Geophysical Lab. The Geophysical Lab will be working in parallel with this proposed effort using lab data and framework theoretical modeling to understand the suite of planetary atmospheric composition types that might be expected before the development of a significant oxygen fraction as occurred for the Earth about 2 Ga.

The objective of this paleoatmospheres subtask is to compile the best available assessments of the atmospheric bulk composition at selected times early in the Earth's evolution. For these periods, we will produce radiatively, thermally, and chemically self-consistent model atmospheres using the integrated chemistry-climate model. The earliest period we will model will be a nominally prebiotic Earth at 4.0 Gyr ago. That environment is thought to have been characterized by higher CO_2 and lower CH_4 than the present day atmosphere. We will also model a late Archean atmosphere (2.8 Gyr ago). For this period we have carbon isotopic evidence for a thriving biosphere with a large methanogenic community, consequently producing a relatively methane-rich atmosphere. After 2.3 Gyr ago, O_2 rose dramatically in the Earth's atmosphere, but the exact amount of oxygen present in a given time period is still contentious. For early atmospheres with oxygen, we will therefore run a suite of models for each period, varying that constituent abundance over a reasonable range. These models will be validated by comparing the predicted surface temperature for a given atmospheric composition, and the known surface temperature for these periods inferred from the geological record.

We will then output the synthetic spectra for a “family of Earths” at different stages in its evolution. For periods known to support life, we will search for potential biosignatures in the spectra, and make assessments of their detectability using the Astronomical Instrument Simulators as described in Task 1.

Biosignatures of a Range of Extrasolar Planets

In this sub-task, we will generate self-consistent solutions for the physical and chemical state of a range of planetary atmospheres with specified surface and exogenic sources and sinks.

For inert atmospheric constituents like molecular nitrogen, the vertical distribution will be fixed in the chemical model. For major source constituents like carbon dioxide, water, and biological emission species (putative biosignatures), the abundances at the lower boundary will be fixed (assuming that the abundance at the surface is buffered by atmosphere/surface processes) or an upward flux will be prescribed. Photochemically-derived minor constituents will have lower boundary conditions reflecting whether or not surface loss occurs. For most planetary scenarios, mass loss to space primarily will consist of escape of atomic or molecular hydrogen, with the lower atmosphere cold trap ultimately determining the limiting escape flux.

Once a thermodynamic and chemical equilibrium state has been reached, we will run tests for the detectability of varying amounts of the *currently accepted* biosignatures. These include H_2O, O_2, O_3, CO_2, CH_4 and N_2O against the bulk atmospheres of modern Earth and representative early Earths that we derived in the previous task. This work will provide an improvement over existing detectability studies in the following areas:

First, all model atmospheres included in this simulation will represent conditions that are radiatively, thermally, and chemically self-consistent. Second, these simulations will generate spectra over the broadest wavelength range possible to facilitate the identification of the most advantageous wavelength regions for detecting these biosignatures. For example, extension down into the near-infrared may be particularly valuable because this spectral range hosts many features from the classic "disequilibrium pairs" of biosignatures, including O_2 and CH_4. Also, features confused by overlap with another spectral feature in the mid-IR may be better separated and observable at near-IR wavelengths. A wide wavelength range will also allow us to probe to different depths in a planetary atmosphere and therefore allow a more comprehensive evaluation of the detectability of biosignatures on the surface and in the atmosphere. For example, mid-IR wavelengths are often sensitive only to a planet's stratosphere, and may therefore provide incomplete information on trace gas abundance, potentially hiding biosignatures

Third, our radiative transfer model can realistically include the effects of clouds on the radiative balance of the planet. Models can therefore include different types of cloud at different levels in a planetary atmosphere and fractional cloud-cover can be simulated with combination of separate runs for a clear and cloudy case. We will therefore also explore the detectability of biosignatures as a function of cloud cover on a terrestrial planet.

Finally, we will run these simulations for a range of different stellar types using realistic stellar spectra, not blackbody approximations. The effect of varying UV fluxes on the photochemistry of the atmosphere, as well as the effects on the insolation can be determined for different stellar types, and the effect on detectability of trace constituents in different wavelength regimes will be explored.

With this study, we will be able to make recommendations on the optimum wavelength and spectral resolution for detection of the currently known biosignatures. However, spectral regions that look promising for biosignature detection from a planetary scientist's point of view may not be quite as appealing when the hard realities of astronomical observing are taken into consideration. While one goal of this project is to simply determine the biosignatures themselves, and then to drive the design of the instrumentation that would be required to detect these, we are also acutely aware of the limitations of the currently proposed first generation of these instruments. Therefore, once the synthetic spectra for this task have been generated, we will first successively degrade the spectra to simulate the anticipated resolutions of future instruments, and to determine at what spectral resolution crucial biosignature information is lost. We will then also run them through the astronomical instrument simulators to determine detectability as a function of instrument detector sensitivity, spectral resolution, aperture size, and against environmental noise factors such as a zodiacal disk.

Statistical Analysis Tools

As part of Task 2, we will also develop a set of sophisticated statistical tools to most efficiently analyze the biosignatures spectral catalog. These tools will provide a probabilistic estimate of the likelihood that a simulated planetary system falls into one of three categories: inhabited, habitable, or sterile, and will allow us to understand and explore the relative importance and interaction of specific features in the model. These database analysis tools are described in more detail below.

Probabilistic Classification of Spectra

Leveraging from work underway on galaxy morphological (Storrie-Lombardi, Lahav et al 1992) and spectral (Ronen, et al) classification, and stellar spectral classification (Storrie-Lombardi et al 1994), we propose to incorporate a set of non-linear, stochastic neural network techniques capable of transforming the multiple data outputs of our model into classifications with co-existent Bayesian probabilities for the correctness of those classifications. Such networks have been previously easily trained to mimic the pattern matching abilities of human experts in galaxy and stellar classification tasks. Their ability to serve as Bayesian estimators makes it possible to attach probabilities to each classification decision in an automated fashion. The algorithms permit the input of multiple data types including (but not limited to) atmospheric spectra and stellar classification of the parent star.

Identifying Critical Biosignature Features

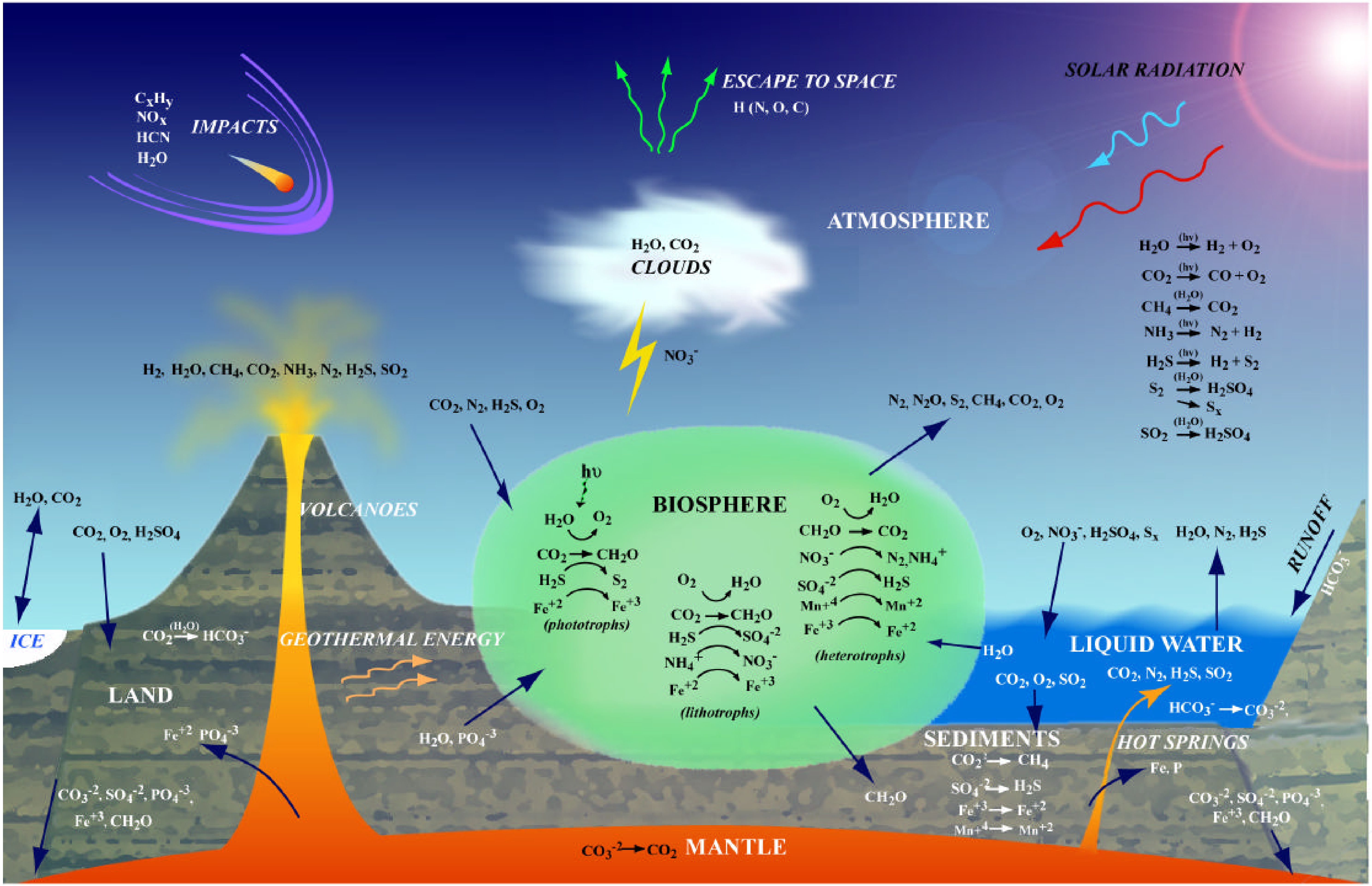
These same non-linear algorithms can be employed to assess both linear and non-linear contributions and interactions amongst the data feature set and have been employed to assess spectral biosignatures (Storrie-Lombardi 1997). The basic technique involves iterative training of a network on data sets devoid of a specific feature or set of features contained in the putative biosignature. For example, the spectra continuum information or specific spectral bands might be removed from training and test sets and the resulting network classification efficiency determined. In other experiments, information about stellar type might be removed. Analysis of both the linear and nonlinear portions of the networks can be accomplished to determine the nature of the interaction between specific features.

C3.3.5 SIGNIFICANCE AND PRODUCTS OF TASK THREE

This task generates the following products:

- Physically, radiatively and chemically self-consistent atmospheres for a suite of Earth's paleoatmospheres based on new constraints provided by laboratory data and geological and biological modeling.
- Physically, radiatively and chemically self-consistent atmospheres for planets around stars other than our own in which abundances of currently identified biosignatures are varied as a test of spectral sensitivity to these constituents.
- Spectra of realistic surfaces and atmospheres (including the radiative effect of clouds and aerosols) produced by the coupled radiative chemical climate model. This work will produce a catalog of spectra, which can be used to characterize the detectability of these biosignatures against a range of atmospheres and for stars of different spectral type.
- Recommendations for detectability of trace gases with no a priori assumptions for instrumentation
- Recommendations for detectability of biogenic trace gases for spectra generated under this task for instruments based on both nulling interferometer and coronagraphic design.
- Development of statistical tools to analyze the resultant comprehensive spectral catalog to determine abundances and best available wavelength regions, sensitivities and spectral resolutions for detection.

As a by-product of this Task, we will produce the best available estimates of the Habitable Zone around stars other than our Sun using a coupled radiative chemical climate model that realistically models the radiative effects of cloud near the limits of the Habitable Zone. The radiative-chemical climate model produced here will be used as the basis for the Abiotic and Inhabited Planetary Models described in the following Tasks.



IMPACTS
C_xH_y
NO_x
HCN
H_2O
ESCAPE TO SPACE
H (N, O, C)
SOLAR RADIATION
H_2O, CO_2
CLOUDS
ATMOSPHERE
$H_2O \xrightarrow{(h\nu)} H_2 + O_2$
$CO_2 \xrightarrow{(h\nu)} CO + O_2$
$CH_4 \xrightarrow{(H_2O)} CO_2$
$NH_3 \xrightarrow{(h\nu)} N_2 + H_2$
$H_2S \xrightarrow{(h\nu)} H_2 + S_2$
$S_2 \xrightarrow{(H_2O)} H_2SO_4$
$\rightarrow S_x$
$SO_2 \xrightarrow{(H_2O)} H_2SO_4$
NO_3^-
H_2, H_2O, CH_4, CO_2, NH_3, N_2, H_2S, SO_2
CO_2, N_2, H_2S, O_2
N_2, N_2O, S_2, CH_4, CO_2, O_2
VOLCANOES
H_2O, CO_2
CO_2, O_2, H_2SO_4
ICE
$CO_2 \xrightarrow{(H_2O)} HCO_3^-$
GEOTHERMAL ENERGY
LAND
Fe^{+2} PO_4^{-3}
CO_3^{-2}, SO_4^{-2}, PO_4^{-3},
Fe^{+3}, CH_2O
BIOSPHERE
hυ
H_2O O_2
$CO_2 \rightarrow CH_2O$
H_2S S_2
Fe^{+2} Fe^{+3}
(phototrophs)
O_2 H_2O
$CO_2 \rightarrow CH_2O$
H_2S SO_4^{-2}
NH_4^+ NO_3^-
Fe^{+2} Fe^{+3}
(lithotrophs)
O_2 H_2O
$CH_2O \rightarrow CO_2$
NO_3^- N_2,NH_4^+
SO_4^{-2} H_2S
Mn^{+4} Mn^{+2}
Fe^{+3} Fe^{+2}
(heterotrophs)
H_2O, PO_4^{-3}
H_2O
CH_2O
O_2, NO_3^-, H_2SO_4, S_x
H_2O, N_2, H_2S
RUNOFF
HCO_3^-
LIQUID WATER
CO_2, O_2, SO_2
CO_2, N_2, H_2S, SO_2
$HCO_3^- \rightarrow CO_3^{-2}$,
SEDIMENTS
$CO_2 \rightarrow CH_4$
$SO_4^{-2} \rightarrow H_2S$
$Fe^{+3} \rightarrow Fe^{+2}$
$Mn^{+4} \rightarrow Mn^{+2}$
HOT SPRINGS
Fe, P
CO_3^{-2}, SO_4^{-2}, PO_4^{-3},
Fe^{+3}, CH_2O
$CO_3^{-2} \rightarrow CO_2$ MANTLE

C.3.4 TASK FOUR – THE RANGE OF PLAUSIBLE ATMOSPHERES FOR ABIOTIC PLANETS

In this task we will determine the range of plausible physical and chemical states for abiotic terrestrial planet atmospheres with active geological and exogenic sources. This study is important to the issue of biosignature detection, because even in the absence of life, a planetary atmosphere can be sustained in a disequilibrium state by a range of abiotic processes. By understanding these abiotic disequilibrium states, we will be able to identify the special disequilibrium states induced by life (Lovelock, 1965; Lederberg, 1965; Hitchcock and Lovelock, 1967; Sagan et al., 1993). This study will also define the range of contexts that result in a habitable planet, and in atmospheric states that might falsely be interpreted as indicating an inhabited planet. Possible "false positives" might include abiotically elevated levels of molecular oxygen, an oxidizing atmosphere with elevated levels of methane, or substantial levels of nitrous oxide.

Current ideas about the climate and composition of lifeless terrestrial planets come from geological records of the early Earth and from present day observations of Venus and Mars. However, it is likely that atmospheres on planets around stars of different spectral type will differ from terrestrial atmospheres in our own solar system. The model proposed here will allow us to explore the abiotic states of a wide range of extrasolar planets.

In this Task we will combine the Coupled Climate-Chemical Model developed in task three with realistic parameterizations of geological and exospheric fluxes to develop the Abiotic Planet Model (APM). This innovative model will provide the most realistic simulation of a terrestrial planet to date.

A planetary atmosphere is a part of a larger planet "system" which includes processes on land and in liquid surface water (if either exists) and in the planetary interior. The volatile composition in the atmosphere is a result of exchange with this system. The carbonate-silicate cycle is a classic example of the connection between atmospheric composition (and in turn the thermal state of the atmosphere) and the other domains (Walker et al., 1981). In a pioneering paper, Hart (1978) documented the factors influencing the size of the Habitable Zone, making use of a computer simulation of the Earth that accounted for a variety of solar and planetary factors and processes, including connections between the atmosphere and interplanetary space, land, ocean, and interior. Schubert et al. (1989) reviewed the processes that couple interiors and atmospheres. Lasaga et al. (1985) and Sleep and Zahnle (2000) provide examples of a mechanistic model simulating cycling of carbon through atmosphere/geophysical domains to yield best estimates for atmospheric composition and its climate implications.

The APM we propose to develop will include more planetary processes than these previous works, including treatments of processes that, in simpler forms, were limitations on the results derived in previous work. The Abiotic Planetary Model is designed to be a testbed for interdisciplinary studies of the factors determining the plausible range of climate and chemistry for extrasolar terrestrial planets and implications for the habitability of these planets. For each computed atmospheric state, synthetic spectra will be generated to support the study of the detectability of biosignatures. The flexible design of the APM will support many collaborations with a wide range of investigators, both scientists associated with the NAI and others in the general astrobiology community.

C.3.4.1 DEVELOPMENT OF THE ABIOTIC PLANETARY MODEL

As illustrated in Figure C.3.4.1, the Abiotic Planetary Model will add two components to the Coupled Climate-Chemistry Model described in Task 3:

- more sophisticated treatments of atmospheric processes at the upper boundary of the model (meteoric influx, and atmospheric escape)
- a mechanistic description of the cycling of volatile constituents between the atmosphere, land, ocean, and planet's interior.

At the upper boundary, detailed simulations of gas escape (particularly hydrogen escape with its impact on the oxidation state of the planet) will be implemented. We will explore the effects of small solar system objects entering the atmosphere—introduction of new material, transformation of the existing atmospheric climate and composition, and erosion of the atmosphere. We will explicitly model the processes controlling the fluxes of volatile species between the

- atmosphere and land (weathering, etc.),
- atmosphere and ocean (air-sea exchange, etc.),
- atmosphere and interior (volcanic emissions),
- land and oceans (runoff and sedimentation), land and the interior (subduction, etc.), and
- oceans and interior (subduction, deep oceanic vents, etc.).

The model also will treat processing of volatiles within the ocean (aqueous chemistry, etc.) and the interior (change in oxidation state of volatiles as a function of oxidation state of interior, etc.). More details on each of these development subtasks will be provided below.

Atmospheric Processes at the Upper Boundary

In this section, we describe atmospheric processes at the upper boundary that will be included as part of the APM. These include volatile escape and impact processes.

Escape of gas to space

The APM will provide improvements over the best existing coupled climate/atmospheric chemistry models (e.g. Brown 1999) by providing improved hydrogen escape formalism. In the Brown (1999) and other existing coupled-climate models, the extent of hydrogen escape is the central determinant of the oxidation state of the atmosphere. However, if hydrogen escape is treated as simple diffusion-limited escape, as it is in these models, overestimates of the extent of hydrogen escape and incorrectly high estimates of atmospheric oxidation can occur. The development of a new, mathematically-tractable hydrodynamic simulation of hydrogen escape as part of the APM advances the current state of planetary modeling.

Gas escape to space from a planetary atmosphere can have two major consequences. First, gas escape can result in reduction in atmospheric elemental composition. The reduction in the nitrogen content of the Martian atmosphere as a result of the non-thermal loss of nitrogen over the age of the planet (Brinkmann, 1971; Nier et al., 1976; Fox and Hac, 1997) is an example of this. Second, the escape of hydrogen from a planetary atmosphere following photolytic dissociation of atmospheric water can result in an increase in atmospheric oxygen, repartitioning elemental oxygen between the source water and the reservoir molecular oxygen without the participation of biology. For example, early in the history of Venus the enhancement of water in the upper atmosphere, and the subsequent photolysis and loss of hydrogen to space, could have produced a transitory high abundance of molecular oxygen (Kasting, 1988).

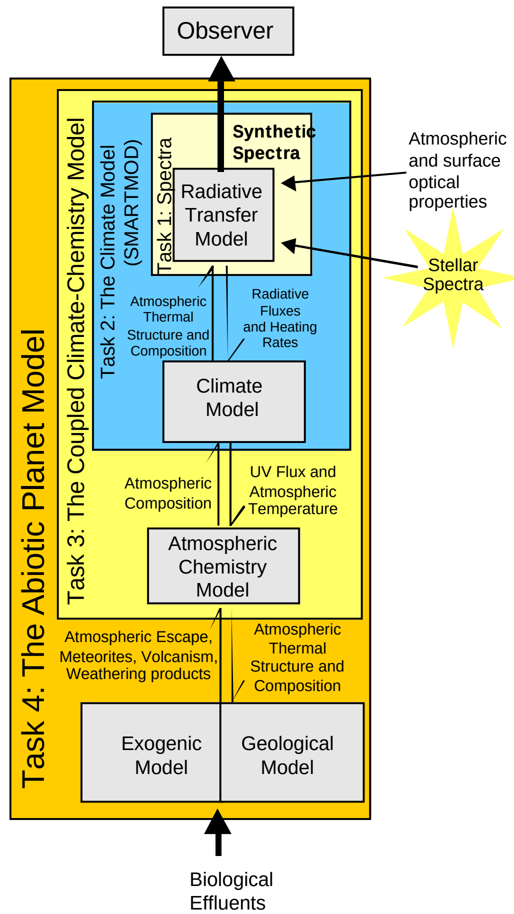


Figure C.3.4.1 The Abiotic Planet Model combines the Coupled Climate-Chemistry Model developed in Task 3 with more sophisticated treatments of gas escape, the effects of impacts, and the cycling of volatiles between the atmosphere and the land, ocean, and planetary interior.

For inclusion in the APM, we will develop a comprehensive model of atmospheric escape. This model will include treatment of gas "evaporation" (or Jeans loss) and hydrodynamic escape of hydrogen where the hydrogen abundances are great enough to generate or contribute to a planetary wind. In the latter case, we will develop an improved treatment that better deals with transonic winds. In both cases, the flow of hydrogen through other (potentially major) atmospheric gases will be considered, including the case of hydrodynamic drag and "blow-off" of heavier species. Non-thermal escape mechanisms will also be treated (which, for example, may be especially important for the evolution of atmospheric oxygen and nitrogen). These non-thermal (ion-exchange, sputtering) processes provide an important example of the coupling between the atmosphere and the interior since the planetary magnetic field plays a role in controlling the non-thermal escape rates.

THERMAL LOSS

Thermal evaporation of gases occurs above the exobase, where the mean free path becomes comparable to the scale height of the overlying atmosphere: particles that attain escape velocity will likely not collide with another particle and will escape. The escape rate can be determined from integration of the upward Maxwellian flux (e.g. Yung and DeMore, 1999). In many cases—including the loss of hydrogen from the current terrestrial atmosphere—the loss rate will be limited by the flow of escaping gas(es) through the non-escaping components. This is diffusion-limited loss and is readily calculated from the diffusion equation for a multi-component gas (Hunten, 1973; Zahnle and Kasting, 1986).

An "evaporative" model of loss is appropriate when a sufficiently small fraction of the velocity distribution of the escaping gas is above the escape velocity that the escaping species does not significantly perturb the vertical structure of the atmosphere. When the loss rates become higher, the gas escapes as a continuous fluid. In this case, the pressure force becomes important (Watson et al., 1981; Kasting and Pollack, 1983), and the loss rate is over-predicted by both the Jeans and diffusion-limited models. In hydrodynamic escape, the escape flux is determined partly by energy considerations and partly by the density of hydrogen at the base of the flow. The escape is powered by solar EUV energy (Watson et al., 1981) and perhaps by interaction with the solar wind as well (Chassefiere, 1996). Sufficiently vigorous hydrodynamic escape can lead to loss of heavier atmospheric constituents. These elements can be dragged or "blown-off" along with the hydrogen, both modifying the atmospheric inventory of heavier elements and modifying the outflow of the "planetary wind" (Hunten et al., 1987; Zahnle et al., 1990; Chassefiere, 1996).

Within the APM, we will treat evaporative escape, diffusion-limited evaporative escape, and hydrodynamic escape, dependent upon the physical conditions of the planetary atmosphere and incident external heating. A major development for this model will be incorporation of a new treatment for hydrodynamic loss. Although "planetary wind" models have been created in the past (Watson et al., 1981; Kasting and Pollack, 1983; Chassefière, 1996), the numerical methods that have been employed to date are not sufficiently robust to allow the incorporation of detailed physics, and to simultaneously explore a broad range of possible primitive atmospheres. Mathematically, one needs to integrate the coupled energy and momentum equations for the escaping gas from the homopause out to infinity. A major difficulty arises because of the existence of a singularity, or critical point, in the one-dimensional, steady-state solution at the distance where the outflow becomes supersonic. Various methods have been applied to provide solutions to the "planetary wind" equations (e.g. Watson et al., 1981; Kasting and Pollack, 1983; Chassefiere, 1996). However, these methods generate solutions which are either ill conditioned, or else provide solutions for a limited subset of cases. For example, Kasting and Pollack (1983) used an iterative method, in which one alternates back and forth between the momentum and energy equations, but were unable to make this work for supersonic solutions. Chassefière (1996) developed perhaps the most elaborate numerical technique, but one that is only valid when the exobase occurs below the critical point, which excludes a whole range of possible H_2-rich primitive atmospheres.

Fortunately, a stable numerical method exists for such problems that allows a generalized treatment of hydrodynamic escape. It is called Godunov's method (Godunov, 1959) and it has been successfully used in one dimension to study "cometary winds" (Gombosi et al., 1985). Godunov's method overcomes the instabilities inherent in modeling subsonic-supersonic transitions by solving shock relations at each grid point instead of using standard finite differences. A detailed description of a first-order Godunov scheme is given by Gombosi (1984). This solution method will be applied to the "planetary wind" energy, momentum, and continuity equations. The interaction between different (escaping and non-escaping) atmospheric gasses will be treated within this system by carrying continuity equations for each species and modifying the momentum and energy equations as composition evolves.

NON-THERMAL LOSS

Non-thermal loss processes involve the ejection of atmospheric gases through interactions with ions or electrons above the exobase, or by photodissociation. Dissociation processes (e.g., electron recombination or electron impact) result in the atomization of molecules, where the resultant atoms may have sufficient velocity to escape. An example of dissociation loss is provided by nitrogen loss from Mars (e.g. Yung and DeMore, 1999). In order to reconcile the observed nitrogen fractionation ratio ($^{15}N/^{14}N$) of roughly 1.62 times terrestrial, roughly 75%+ of the original atmospheric nitrogen must have been lost (Fox and Hac, 1997). Similar dissociative loss of oxygen should have occurred, but no fractionation relative to terrestrial is observed, suggesting that oxygen is buffered by a large, non-fractionated oxygen reservoir (Owen, 1992).

Impact of energetic ions and atoms provides an additional loss process. Solar wind particles are capable of removing ("sputtering") hydrogen molecules, and compete with Jeans thermal loss in the current terrestrial atmosphere (Hunten et al., 1989). A related process, indirect solar-wind induced sputtering, can eject heavier species and will likely be important on planets without a magnetic field. Here, EUV produced O^+ ions are accelerated by the draping of the solar wind magnetic field over the ionosphere. Some of these ions are directed back into the atmosphere, where they impact molecules and/or atoms, providing some with sufficient energy to escape (Luhmann et al., 1992; Kass, 1999). Such sputtering models have been used to estimate loss rates for CO_2 from the Martian atmosphere (Kass and Yung, 1995, 2000) resulting in loss estimates of between 0.2 and 0.8 bars of CO_2 (as compared to a current atmospheric inventory about $6x10^{-3}$ bars).

For the APM, we intend to incorporate dissociative recombination and particle impact loss mechanisms. Treatment of dissociative recombination will follow Fox and Hac (1997). The production of candidate loss ions in the upper atmosphere, as well as the structure of the upper atmosphere, will be calculated by the APM photochemical and radiative models and passed as input to the loss model (following a similar approach as Fox, 1993). Based on these distributions, the dissociative recombination yields will be calculated and used as input for a Monte Carlo loss calculation (Fox and Hac, 1997). These calculations use Maxwellian initial velocity distributions and random initial directions to calculate loss probabilities and hence rates. While Fox (1993) and Fox and Hac (1997) concentrated on nitrogen, we will also treat oxygen loss.

Treatment of sputtering will follow Kass (1999). Again, the composition and structure of the upper atmosphere will be taken from the APM photochemical and radiative models. In this case, a model for the incident O^+ ions is required, which depends strongly on the assumed planetary magnetic field. Given a magnetic field produced by the geophysical (interior and planetary formation) model, we will use the work of Luhmann et al. (1992) and Luhmann and Kozura (1991) to estimate O^+ production and impacting populations. The Monte Carlo sputtering model then "follows" the incident oxygen ion and maps impact histories using a library of impact cross sections.

Effects of impacts

Depending on the size of an object entering a planetary atmosphere, the impact can chemically modify or add to the target atmosphere by the reprocessing (mostly by shock heating) of air already present, by the ablation of new exogenic material from the impactor, or by volatilization of planetary materials (e.g., it can liberate CO_2 from carbonate rocks, or it can evaporate water). Some classes of impacts can remove more volatiles from a planet than are added. The objective of this proposal activity will be to develop globally averaged rates for atmospheric processing as a function of the flux and composition of impactors.

ATMOSPHERIC MODIFICATION

Impacts can change the chemical speciation of the existing atmosphere either by shock heating air or by directly reacting with the air. In a strongly shock-heated gas, temperatures get so high that ordinarily stable molecules react to form a thermochemically equilibrated mix; rapid cooling of the gas leaves many chemical species "quenched" at relatively high abundances, far from equilibrium because their destruction is kinetically inhibited. The disequilibrium products that survive depend most strongly on the elemental composition of the shocked gas. A general rule of thumb is that CO forms until either C or O is exhausted. If O>C, oxidized species result, if C>O, reduced species result. Impact shock chemistry has been addressed as a source of nitrogen oxides in a modern terrestrial atmosphere (Prinn & Fegley 1987; Zahnle 1990) and as a source of HCN in more reduced atmospheres (Fegley et al. 1986, Fegley & Prinn 1989, Chyba & Sagan 1992).

Methods developed elsewhere for impacts on Earth (Zahnle 1990; Toon et al 1997) and for impacts on Jupiter (Zahnle 1996) can be applied to impact shock chemistry in atmospheres in general. For impacts on planets with solid surfaces, there are 4 major shock processes:

- the inbound passage of the impactor through the atmosphere;
- the expansion of the ejecta plume through the atmosphere;
- the reentry into the atmosphere of ejecta; and
- radiative heating of the entire atmosphere and surface.

These processes become progressively more important in the order listed as the impact energy is increased.

The first process is relatively well understood (Park and Menees 1978). For objects small enough to stop in the atmosphere, we can approximate each individually by a terminal explosion that processes a predictable amount of atmosphere at an altitude above a quench temperature. These objects will contribute ablated vapors to the atmosphere according to the impact velocity and the chemical composition of the impactor. Objects large enough to reach the surface without slowing down deposit relatively little energy or ablated material into the atmosphere before they hit the ground. The net effect on the atmosphere of the first process can be usefully approximated by global average rates as functions of altitude.

The second process is more important because it harnesses a greater fraction of the energy of the larger impacts (Prinn & Fegley 1987). Zahnle (1990) used an analytical approximation suggested by Zel'dovich & Raizer (1967) to model the superheated rock vapor (and/or water vapor) ejecta plumes to estimate the mass of strongly shocked air. The amount of atmosphere shocked above a given quench temperature is computed from the momentum of the ejecta plumes. As with the first process, the effect on the atmosphere can be usefully approximated by global average rates.

Examples of the third process are provided by the 1994 impacts of comet D/Shoemaker-Levy 9 with Jupiter and the leading model (Melosh et al. 1990) for starting global wildfires at the K/T boundary. Air can be shock heated either by gas-on-gas shocks as the plume falls or by reentry of myriad tiny ejecta particles. Zahnle (1990) used this model to estimate NO production for the K/T impact. For impacts of this scale, it is most useful to regard the materials of the impactor itself as being dispersed at the highest ejecta velocities. Much of this will escape if these are high enough. The SL9 events provided an opportunity to test models of impact-induced atmospheric chemistry. Zahnle (1996) devised a chemical kinetics model for the H, N, C, O, S system appropriate to SL9. The model traces the evolving chemical composition of a parcel of gas by directly integrating the web of chemical reactions. Pressure and temperature histories of the parcels are modelled after those calculated by numerical hydrodynamic simulations of the ejecta plume. In general, a given parcel is shocked twice; i.e., a parcel strongly shocked near the impact site is ejected at high velocity and is therefore shocked again when it reenters the atmosphere. Hence the final state of the gas often depends on the second shock. Shock products are computed for a range of different peak shock temperatures, ejecta velocities, and chemical compositions. The latter can include material from the impactor.

The fourth process only becomes important for the largest impacts. Essentially the entire atmosphere is radiatively heated by infalling ejecta, and so the atmosphere is globally "reset". For Earth's present atmosphere this occurs for events comparable to the impacts that formed the lunar Orientale and Imbrium basins ca. 3.8 Ga. There were hundreds of similar impacts on Earth ca. 3.8-4.2 Ga, and thus all four process are likely to affect inhabited planets.

To put impacts into an atmospheric chemistry code requires that we specify the effects of shock-heating of ambient air as well as the chemical content of the impactor. Because high altitudes are affected more often than low altitudes, and because more air is processed at low temperatures than at high temperatures, the most useful description of shock heating of ambient air is to specify how often the atmosphere above a certain altitude z gets heated above a quench temperature T. Quench temperature is a weak function of the cooling time scale, but it is sensitive to chemical composition and will need to be specified according to air composition. Photolytic chemistry driven by thermal ultraviolet radiation can be important to lightning in some atmospheres, but is less likely to be important in impacts because radiating temperatures in impacts are much lower. Vapor ablated from the impacting bodies themselves can also influence the redox budget of the atmosphere (Kasting 1993); this effect will also be included in the atmospheric chemistry model.

IMPACT EROSION.

Impacts cannot be regarded solely as a source of volatiles. Provided it is big enough and energetic enough, an impact can expel more volatiles from a planet than it adds. A popular example in this solar system is the planet Mars, for which the leading hypothesis is that its atmosphere was mostly stripped by impact erosion (Melosh and Vickery 1989). The mass of atmosphere stripped by impacts depends upon the velocity of the impactors, the size of the planet, and the size of the impactors. The dependence on planetary size is illustrated by the analytic fit to numerical calculations derived by Melosh and Vickery (1989). Above a specific impactor mass, which is determined by the atmospheric pressure and scale height, as well as the planetary radius and gravity, all the atmosphere above the impact tangent plane is lost. However, there is some disagreement over how efficient impact erosion actually is. Walker (1986) suggest that only air directly interacting with the bolide will be ejected, while Newman et al. (1999) use numerical models to show that only the “entry column” of atmosphere is significantly accelerated. In the proposed work, we will use descriptions of impact erosion described by Zahnle et al (1992) to address the efficiency with which atmospheres are supplied or lost as a function of planetary parameters (escape velocity, principally) and of the parameters describing the population of impactors (composition and impact velocity, principally). Zahnle et al. (1992) considered both aggressive impact erosion as proposed by Melosh and Vickery, and the less aggressive forms of impact erosion proposed by Walker (1986) and Ahrens and O'Keefe (1987).

IMPACT FLUXES

The problem of impact flux populations is a significant one. Ideally, we would simulate the impacting flux populations as a function of the star and the location of the planet in the system. However, the credibility of such an effort would be dubious given the observational constraints. Instead, we can take a number of different approaches. The lunar record of impacts provides an impactor flux history that is scaled and applied throughout the solar system (e.g. Melosh, 1989; Neukum and Ivanov, 1994). Insofar as this represents an impactor flux for a system consisting of a mix of terrestrial and gas-giant planets, we will used a scaled version of this flux to generate the individual impactor consequence results for generation of atmospheric histories (see above). The lunar impact record can be used to construct a chronology of impact intensity because surfaces of different ages, with differing crater densities have been geochemically dated. For a given crater size range, the cumulative impact density on a surface can be derived as a function of age. For example, Neukum and Ivanov (1994) provides an analytic formulation that can be differentiated to give an impact rate function which decays exponentially. Lunar and planetary impact craters also provide some constraints on impact size distributions. The distribution appears to follow a power law with exponent of -3 for <4km (Neukum and Ivanov, 1994). Estimates of size distributions of near-Earth crossing asteroids provides an additional source of information. Rabinowitz (1993) finds a power law of -5.4 for > 3.5 km, increasing to -3.5 to -2 for smaller objects. However, the lunar impact flux history and near-Earth asteroid populations are likely strongly affected by the specific arrangement of our solar system, most directly to the existence of Jupiter at its location. To test the sensitivity of results to the chosen impactor record, we will use the impacting flux history as a free parameter.

Geophysical Cycling of Volatiles

The Earth provides an initial analog for the interaction of solid planetary surfaces with planetary oceans and atmospheres. Research on this topic involves many branches of Earth Science. We can extrapolate to other planets by examining how terrestrial geochemical cycles work and how conditions elsewhere are similar to or different from those on the Earth.

Much can be learned about the Earth simply by considering the size of reservoirs and the magnitude of the fluxes between them. It is convenient to divide planets from top down into atmosphere, ocean, crust, mantle, and core, with some grouping and subdivision. Since the core interacted chemically with the rest of the Earth only during its formation, we define the global reservoir of an element to exclude the core. The crust and mantle are the silicate part of the Earth. Crust, ocean, and atmosphere are shallow geochemical reservoirs; sedimentary rocks, ocean, and atmosphere are surface reservoirs.

The mantle is about 2/3 of the mass of the Earth compared with 0.05% for the shallow reservoirs. However, some biologically significant elements are strongly concentrated in the shallow reservoirs. A sizable global fraction of the global H, C, N, and Cl are in various surface reservoirs. Ocean water is the dominant reservoir for H and Cl. The atmosphere is a significant reservoir for N and rare gasses. Sedimentary rocks contain massive carbonate deposits. S and P, in contrast, have remained mainly in the mantle. Their abundance in surface reservoirs is limited by the rate that they are liberated, ultimately from plentiful quantities in igneous rocks, by weathering and by hydrothermal circulation. That is, there is plenty of P and S in reasonable igneous rocks.

We discuss two specific issues in more detail to show how our understanding of the Earth and other solar planets can be used to infer conditions elsewhere. We begin with the chemistry of igneous rocks. The global carbon cycle is an example where the efficacy of crustal traps determines the partitioning between the mantle and surface reservoirs.

Composition of reactable igneous rocks.

Weathering of rocks on land and the hydrothermal circulation at depth involve rock/water chemical reactions. Vented fluids and altered rocks at oceanic and land sites have been extensively studied. The long term composition of the ocean and the atmosphere are determined by such reactions, and by reactions that follow the depostion of sedimentary rocks.

The most abundant igneous rock on the surface of the Earth is the mid-ocean ridge basalt (MORB), which upwells from the mantle and covers the floors of the ocean basins (60% of the Earth's area). Massive amounts of hydrothermal circulation through the basalt occur near midoceanic ridge axes. The process has significant effects on the chemistry of the modern ocean. For example, there is a net flux of Mg into the rock and a net flux of Ca into the water. The basalt becomes somewhat oxidized, removing dissolved O_2 and sulfate from the water. As discussed below, the erupted basalt carries CO_2 from the mantle to the surface and later becomes carbonatized so that subduction returns CO_2 to the mantle.

The composition of the silicate mantle ultimately is determined by the composition of the stellar nebula out of which a planet forms. This is not planet specific. Basaltic rocks are expected to be the dominant rock type in terrestrial-class planets with modest variations in composition. Sampling within our solar system indicates that this is true.

Global carbon cycle.

The terrestrial carbon cycle couples the atmosphere to interior processes. Its surface reservoir, mainly sedimentary carbonates, has a limited capacity. On an abiotic planet, carbonate can be sequestered in both shallow water and deep water.

The effect of atmospheric CO_2 on climate has been studied extensively. It has been suggested that a clement climate has always required high levels of atmospheric CO_2 (Owen et al., 1979, Kasting, 1993), but the evidence from the geological record prior to 2.2 Gya appears not to support this hypothesis (Rye et al., 1995). Sleep and Zahnle (2000) present a new argument, based on CO_2 fluxes in to and out of the mantle, that weighs against high levels of CO_2 on early Earth during the Archean and the Hadean eras.

In the carbon cycle, there are five significant reservoirs: the atmosphere, free carbonate in the ocean, carbonates lying upon or veined within oceanic basalt, carbonates on continental platforms, and CO_2 in the mantle. Of the vast amount of terrestrial CO_2 that is not in the atmosphere, roughly 6×10^{21} moles are currently in the crust and a comparable or larger amount is in the mantle (e.g., Zhang and Zindler, 1993). The current CO_2 mantle outgassing rate, ~2.5×10^{12} moles/yr (ibid.), is fast enough to double the surface carbonate inventory in 2.4 billion years, and the mantle connection would have been stronger during the Archean. To first approximation, under plate tectonics ocean crust is recycled as the square of the heat flow. On early Earth, with a geothermal source 2-3 times that of today, ocean crust would have been created and subducted 4-9 times faster than today. Outgassing increases proportionately, so that the time scale for doubling crustal carbonate drops to 300-700 Ma. Evidently the mantle cannot be neglected on Earth's longest time scales. In particular, ingassing is needed to close the mantle cycle. Possibilities include subduction of carbonates directly deposited on the ocean floor (pelagic carbonates); subduction of continental carbonates that are scraped off and dragged down; and subduction of carbonates formed by seawater alteration of the oceanic basalt itself. The latter in particular depends on the amount of free CO_2 in the ocean, and hence can act as a buffer on atmospheric CO_2 levels. The atmosphere and ocean are linked by the effective solubility of CO_2. There are currently 6.2×10^{16} moles of CO_2 in the atmosphere and 3.3×10^{18} moles in the oceans; the ratio is 54:1. These reservoirs are tightly coupled on geological time scales, so that the air is refreshed in a thousand years.

Sleep and Zahnle (2000) have modeled the carbon dioxide cycle, focussing on the mantle reservoir and the exchange between surface reservoirs and the mantle, using the language and concepts of plate tectonics to extrapolate the CO_2 cycle into the past. Their first step is to construct a specific albeit much-simplified model of the modern CO_2 cycle as the Earth's CO_2 cycle is complicated and not fully understood. For purposes of presentation, they organize their reservoirs and fluxes following Tajika and Matsui (1992). They use arc fluxes modified from Plank and Langmuir (1998) and Sano and Williams (1996) and ridge fluxes from Zhang and Zindler (1993). They then accelerate the cycle into the Archean, taking into account the greater influence of the mantle and the diminished influence of the continents. Finally, they consider the effects of abundant impact ejecta on Hadean cycles.

The flux equations are then solved numerically. The procedure for modeling other real or hypothetical planets is similar. To illustrate the parameterization procedure, we discuss fluxes at midoceanic ridges.

The flux of CO_2 from the mantle to ridges is an example where the flux depends only on interior processes. At the relatively shallow depth where midoceanic ridge basalt forms, CO_2 is nearly quantitatively extracted from the mantle into the magma. Most of the CO_2 down to about 56 km (Langmuir et al., 1992) is extracted. The basalt ascends to crust depths where most of the CO_2 escapes into the ocean. The CO_2 concentration in modern magmas is estimated from He/CO_2 ratios and the known flux of He into the ocean. The mantle concentration then obtained has the average fraction of melting known independently of CO_2. The process in the past differed from that of the present in that the mantle was hotter causing the extraction depth to be greater and the mantle reservoir was probably larger, as less CO_2 was within crustal carbonates.

In contrast, the CO_2 from the carbonatization of midoceanic ridge lavas by hydrothermal circulation depends on shallow processes and the concentration of CO_2 in the ocean. That is, the amount of CO_2 taken up in the rock depends on the oceanic concentration (to a power less or equal to 1). The amount of water circulated through a given surface area of oceanic crust is expected to change little over time. The magnitude of the modern flux is calibrated by monitoring the composition a vented water which reacted with the rock and the composition of reacted rock samples.

This model is a traditional treatment of climate buffering via the update of CO_2 by weathering of silicates on land if the mantle cycles are ignored. However, mantle fluxes are important over long geological times. The dependence of CO_2 flux from carbonatization of oceanic basalt on the amount of it in the ocean and hence the amount of it in the air acts as a buffer. Cold climates are expected particularly early in the Earth's history unless another greenhouse gas was important.

Modeling of any planet with an ocean is analogous to the Earth, although planets with no large standing bodies of water can also be modeled. The ground water in the shallow subsurface can be treated either as part of the mantle box or as a separate shallow box closely coupled to a deeper mantle box.

Modeling the cycling of other volatile species

A mechanistic model of the cycling of carbon will be similar to the approaches taken by Lasaga et al. (1985) and Sleep and Zahnle (2000). The abiotic version of the water cycle (see below) also will be implemented. The analysis for nitrogen is similar to that for H2O: both have a long residence time in surface reservoirs.

Time-dependent planetary evolution scenarios

The coupled planetary system intrinsically varies with time due to as number of factors. The brightness of the central star varies as it ages. The planet interior cools with time. The character of the impact flux changes with time and, in particular, large, planet-altering impacts may occur only once in a planet's history.

Consequently the Abiotic Planetary Model will produce time-varying planetary evolution sequences, forced by the natural variation of stellar and planetary processes. For example, in the carbon cycle which will be based on the Sleep and Zahnle (2000) model, there are time-dependent specifications for mantle degassing, ocean basalt hydrothermal circulation, subduction rate, subduction efficiency, continental metamorphism, and solar luminosity.

Since the model will be a time-dependent simulation, we will be able to investigate the consequences of singular events in a planet's history such as a major impact.

Model validation

The ability of the Abiotic Planetary Model to simulate what is known about the physical and chemical state of the atmosphere of the early Earth and also the current states of the atmospheres of Venus and Mars serves as the key validation test of the APM.

Venus and Earth seem to have comparable amounts of carbon dioxide and nitrogen, taking into account the carbonate reservoir on the Earth. It is not unreasonable to consider that both planets formed with comparable amounts of water. At the elevated temperatures corresponding to its closer position to the Sun, the early Venus upper atmosphere could easily be more humid than the case for the Earth. With more water in the upper atmosphere, the loss of hydrogen to space is enhanced sufficiently to lose the planetary inventory of water. In the absence of water, the processes that transform atmospheric carbon dioxide to carbonate would be much suppressed on Venus relative to the Earth situation, sustaining the high atmospheric abundance of carbon dioxide.

Mars also may have started out with amounts of carbon dioxide and water comparable to the Earth's. Being smaller than the Earth, Mars's gravity cannot hold atmospheric gases from escaping thermally or non-thermally as effectively as the Earth can. Also a result of the smaller planetary radius, the interior of Mars has cooled sufficiently to shutdown tectonic activity. If tectonic activity subsided while Mars still had a warm, humid atmosphere, the atmospheric burden of carbon dioxide would be converted to carbonate, but recycling back to the atmosphere would be suppressed. In time, the Martian atmosphere would drop to the level observed today.

These scenarios that explain the current differences between the atmospheres of Venus and Mars and that of the Earth, considering that these three terrestrial planets may have had initial atmospheres very similar to that for the early Earth, provide a good opportunity to test the Abiotic Planetary Model. The validation tests are designed to confirm that the processes in this model controlling the partitioning of volatiles amongst the atmosphere, land, ocean, and interior domains are a reasonably complete set and that the parameterizations have some appropriate level of realism. One experiment would be to move an early Earth to the distance of Venus and see if the computed atmosphere relaxes to a physical and chemical state similar to what is observed today for Venus. Does the model produce a "runaway greenhouse" or a "moist greenhouse," which in either case increases the atmospheric water content, enhances loss of hydrogen to space, and diminishes the surface water reservoir?

A second experiment would be to move an early Earth to the distance of Mars from the Sun and scale down the planetary size to that of Mars. The test then would be to see that the APM so initialized would relax to the atmospheric state currently observed on Mars. To what extent is impact erosion necessary to explain today's thin Martian atmosphere?

Successfully demonstrating that the APM provides a reasonable simulation of the planetary-scale cycle of volatile species for the three terrestrial planets in the Solar System sets the basis for use of the APM to model "terrestrial" planets in other solar systems.

C.3.4.2 RESEARCH TASKS

Once validated, the APM will be used to explore the range of plausible atmospheres for a wide variety of extrasolar planets to address the issue of "false positives". Specific experiments and questions we will address using this model would include:

· Determining the range of molecular oxygen abundance in an extrasolar planet atmosphere that can be produced by abiotic sources. A planet with a CO_2 atmosphere and little water can have a large fraction of O_2 (Nier et al., 1976), especially if a planet is larger than Mars and oxygen escape is suppressed. A planet such as an early Venus with a lot of water vapor in the atmosphere and, in the presence of intense stellar ultraviolet radiation, may have an especially O_2-rich atmosphere following the escape of hydrogen (Kasting, 1997). How long would the O_2-rich atmosphere last?

· Can any abiotic planet have detectable levels of both CH_4 and O_2 (or the O_3 proxy)?

For atmospheric compositions and surface properties derived from these model runs, we will also output high resolution synthetic spectra and assess these spectra for detectability of spectral features using the instrument simulators and statistical methods developed in Tasks 1-3.

Additional Research Tasks

In addition to the principal tasks described above, there are a number of other investigations that will be supported by the APM. As time permits, we will run as many of these experiments as possible.

· Model planets for a range of central star stellar types, considering a range of planetary size, composition, rotation rate and obliquity , impact history, H_2O inventory (follow through on consequences of H_2O and CO_2 clouds and UV-shielding photochemical hazes).

· Can a planet warmup from a cold start? I.e., the planet starts out frozen (surface frozen with CO_2 clouds) at low stellar flux, but because of its high albedo the planet might not warm up when stellar flux increases (Kasting 1991, Caldeira and Kasting 1992). However, clouds also might produce warming (Forget and Pierrehumbert, 1997). What about warming from a massive impact or extensive volcanism?

· The sensitivity of planetary evolution to the initial volatile inventory. If the initial water content of a planet is half that of the Earth, there might be no surface water. If double that of the Earth, there might not be any continents. In the later case, the carbonate cycle might still be possible with aquatic chemistry, but much slower.

· To what extent can a single impact significantly change the volatile inventory of a planet? Is a planet with enough water to be habitable just a coincidence?

· With reduced solar flux levels, CH_4 will have a longer lifetime relative to photolytic decomposition. At low stellar luminosities, can a tectonically active planet with a reduced mantle produce enough methane to maintain a clement environment?

· How big would a planet have to be to retain its H_2 inventory and remain in a reduced oxidation state for its whole lifetime?

· The sensitivity of climate to the N_2 abundance. More N_2 on the Earth would moderate daily temperature fluctuation. Less of it would cause nightly frost. It appears that N_2 behaves like H_2O in the sense that only so much can go into the mantle. Like hydrogen, nitrogen is more abundant in the accreting material than it is in the final silicate plus surface reservoirs of the Earth.

· What is the lower size limit to a habitable planet? Is this limit restricted to a sufficient size to maintain the carbonate-silicate cycle that is thought to be the key to clement climate stability (Walker et al. 1981, Kasting 1988)?

· Role of impacts in allowing any particular planet to be habitable. How can a major impact lead to a deviation from the planetary evolution sequence?

· At what planetary distances from a central star, do moist and runaway greenhouses suppress a habitable planetary state for a given solar flux? Previous work (Kasting et al. 1993) parameterizes clouds with high surface albedo, rather than the more realistic treatment in the APM. Real clouds may allow surface water at higher solar flux (Chyba et al., 2000).

· Outer limit of Habitable Zone: how far out can a planet the size of the Earth remain habitable? a planet the size of Mars? To properly address this question, one needs a realistic treatment of CO_2 clouds (Chyba et al., 2000).

· For faint stars, would planets have to get so close to be habitable that they end up tidally locked? Then without a day/night cycle and if there is only a thin atmosphere, a planet might be frozen on one-side (Joshi et al. 1997).

· To what extent is the range of the Habitable Zone around a specific stellar type changed if one considers an expanded definition that includes the presence of liquid water at some depth below the surface (Chyba et al., 2000)? Sub-surface life could survive intense stellar radiation. On Earth there is a subsurface biosphere feeding off geothermal energy, not surface photosynthesis.

C.3.4.3 PRODUCTS AND SIGNIFICANCE

The Abiotic Planetary Model is a tool for investigating the variety of planetary climates and atmospheric composition that can arise from a combination of stellar type and planet context and provides a valuable tool for furthering our understanding of the Habitable Zone.

This task will produce a comprehensive suite of physically, radiatively and chemically self-consistent atmospheres for a range of uninhabited planets. We will analyze the synthetic spectra produced to investigate the relationship between spectral features and the climate/chemistry of a planet, and determine what features unique to a particular planetary state are detectable.

We will also use modeling results for a range of abiotic planets around stars other than our own Sun to determine the plausible range of atmospheric compositions for abiotic planets. We will then determine the likelihood of "false positives", abiotic planets that may produce spectral signatures that could be mistaken for life. We will also determine what combination of auxiliary parameters, if any, should be looked for to remove the potential ambiguity in these cases.

The APM will be a multipurpose tool for use by the science team and a forum for collaborations between the science team and NAI member scientists and members of the broader astrobiology community. The APM will be programmed in a modular fashion to allow easy exploration of alternative formulations of processes integrated in the APM simulation of a planet.

C.3.5 TASK FIVE—THE INFLUENCE OF BIOLOGY ON THE COMPOSITION AND SPECTRA SIGNATURE OF AN EXTRASOLAR PLANET

The objectives of this task are to determine the unique attributes of a habitable terrestrial-type planet that result from the presence of life and the detectability of these attributes by remote-sensing spectroscopic observations.

To address these objectives we will add processes involving life to the Abiotic Planetary Model developed in Task 4 to create an Inhabited Planetary Model (IPM). For each simulation of a planet with life, synthetic spectra will be generated to determine whether the influences of biology on the observable environment are detectable. As with the APM, the IPM has a flexible design that will allow it to support many collaborations with a wide range of investigators, both scientists associated with the NAI and others in the general astrobiology community.

C.3.5.1 DEVELOPMENT OF THE INHABITED PLANET MODEL

Life can affect the observable planet— atmosphere and surface —by mediating the cycling of volatiles between the atmosphere and land, water, and interior. One example of this is the role life can play in the carbonate-silicate cycle discussed in detail in Task 4. Plants can enhance the partial pressure of CO_2 in surface soils, accelerating the formation of bicarbonate, and can enhance the rate of carbonate precipitation in the oceans through the secretion of plankton shells, for example. We will augment the Abiotic Planet Model developed in Task 4 with a suite of biospheric processes to develop the Inhabited Planet Model (Figure C.3.5.1). Figure C.3.8 (pg. 34) now illustrates the range of processes that will be addressed in the Inhabited Planet Model.

The following sections describe in detail the life processes that will be parameterized and added to the APM to produce the IPM. These are broken into two principal subclasses: geophysical-biological cycles, and the direct effect of life on an atmosphere.

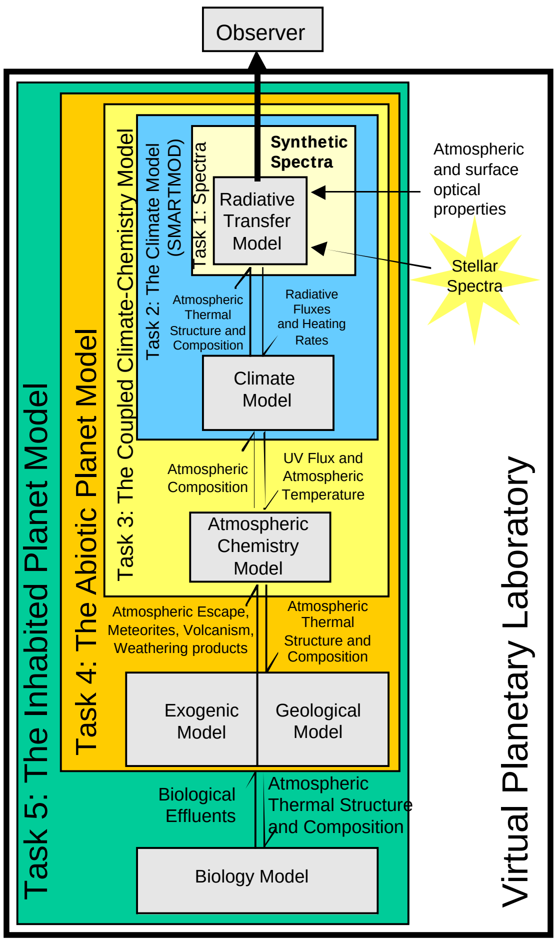


Figure C.3.5.1. Components of the Virtual Planetary Laboratory included in Task 5 are shown. The Abiotic Planet Model is augmented with biological processes to produce The Inhabited Planet Model.

Geophysical-biological cycles of volatiles

The mechanistic descriptions of cycling of volatile species between the atmosphere and land/ocean/interior will be expanded to include processes introduced by the presence of life.

The global water cycle is an example where the mantle reservoir can hold only so much of an element and is an example of coupling with the surface oxygen cycle. In this case, the oxygen cycle is fundamentally biological, while life does not grossly effect the water cycle. Even within the habitable regions of the Earth's crust (including soils), biology serves mainly to speed up chemical reactions which would occur anyway. Consequently, some of the processes discussed here will be treated in the mechanistic model developed for the APM (Task 4).

In some cases biological processes can dynamically overwhelm the buffering of the ocean and atmospheric composition. In regard to the Earth the issue of how atmospheric O_2 is maintained when it is grossly out of equilibrium with the FeO within igneous rocks is of interest because there is no sufficient abiological source.

The gross features of our oxygen atmosphere are well known. The O_2 which we breath has built up over geological time from photosynthesis, which is simply expressed as the reaction: $CO_2 \rightarrow C + O_2$. The burial of organic carbon within sedimentary rocks has inhibited the back reaction to CO_2 allowing O_2 to persist in the air. A global microbial ecology, where the back reaction went to near completion, worked fine on the early Earth.

Using the Earth as the best available analogue gives the chain of linked processes that lead to reduced carbon burial. Around 70-80% of the reduced carbon in terrestrial sediments is in shales (Holser et al., 1988). The reasons for this are fairly evident. Shales form from deposits of clay-rich mud. They are relatively impermeable, preventing extensive contact with circulating oxygen-rich surface waters. Shale beds retard the circulation of water into interbedded sandstones and limestones, protecting the remainder of the reduced carbon in sediments.

The ultimate source of shales is Al-rich igneous rocks. Significant Al_2O_3 is present in most common igneous rocks and clays form from their weathering. The complicating factor is that FeO consumes oxygen by the reaction, $4FeO + O_2 \rightarrow 2Fe_2O_3$. The mantle derived mafic rocks, basalt and gabbro, have about 10% FeO and 15% Al_2O_3, while continentally derived granites have only 2% iron as FeO (some of which is already oxidized) and 15% Al_2O_3 (Krauskopf and Bird, 1995). The basaltic sink is potentially significant given that seafloor spreading renews the oceanic crust every 100 m.y. For example, there is enough FeO in the uppermost kilometer of the oceanic crust to consume 3×10^{20} moles of O_2. This compares with the 0.4×10^{20} moles of O_2 in the air (Garrels and Perry, 1974). Other surface reservoirs of free oxygen are more massive. Fe_2O_3 in sedimentary rocks comprises the equivalent of 1×10^{20} moles of O_2 and sulfate in the ocean, and sediments comprise the equivalent of 4.8×10^{20} moles (Garrels and Perry, 1974). Oxidation of the uppermost kilometer of oceanic crust would remove the O_2 and sulfate reservoirs in under 200 m.y. A significant amount of ridge basalt has in fact been altered over geological time to form Fe_2O_3, which was eventually subducted. This process has left more reduced carbon in sediments, equivalent to 10.4×10^{20} moles of O_2, than the sum of the surfacial free oxygen reservoirs (Garrels and Perry, 1997). Conversely, the small relative size of the atmospheric O_2 reservoir indicates that subtle variations in the basalt/granite ratio of sedimentary sources could have profound effects.

For the present situation to occur, granite, which makes clays, must dominate over basalt, which removes O_2, in the global (igneous) sedimentary source. That is, continents, where granite is a significant rock type, were exposed to weathering and erosion to a much greater extent than mid-oceanic ridges, which are mostly basalt. There seems to be just the right amount of water in the Earth's oceans. Much more would cover all land precluding erosion and much less would leave the ridge axes exposed. Increasing or decreasing the global surface volume of water by a factor of 2 would greatly change the Earth's surface and a factor of 4 would render it unrecognizable.

The amount of water for each case is obtained because the elevation distribution is known on the Earth (Sandwell and Smith, 1997). The current ocean is equivalent to a 2.5-km thick global layer and ~1/10 of this amount is buried in sediments. Beginning with the amount of water needed to cover dry land, the highest large uplifted region on the Earth is the Tibet plateau with an elevation of 5 km; the Altiplano has 3-km elevation. Adjusting for the load of the water, an additional 7-km thickness of water would cover Tibet. Only 3.8% of the Earth's surface is above 2-km elevation. An equivalent water layer of 1.1-km thickness lies beneath the current ridge axis. Further reducing the global amount of water to an equivalent area of a few hundred meters would produce conditions like early Mars where the bulk of the water at any one time was buried in sediments.

Surface topography is the result of the combined effects of tectonics and erosion by water. The topography in turn has a significant influence on climate, for example, the amount of rainfall, and ultimately impacts the composition of water runoff from the land mass to the ocean.

The surface plus mantle reservoir of water was determined by processes during accretion of the planet. The mantle can accumulate only so much water and the rest ends up in the ocean. Water degasses at midoceanic ridge axes at a rate proportional to the amount in the mantle. Hydration and eventual subduction of oceanic crust returns water to the mantle. A fraction of the water is deeply subducted and the remainder is returned to the surface at island arc volcanoes. Higher mantle temperatures enhance degassing, while lower temperatures favor deep subduction of water.

The steady state amount of water in the mantle is independent of the global spreading rate and should increase in time as the Earth's interior cools. The time to reach steady state depends on the time to circulate the volume of the mantle through the melting regions of midoceanic ridge axes, which now extend to a depth of ~56 km (Langmuir et al., 1992). This time is now quite long as can be seen from the behavior of argon.

Viewed in a more sophisticated way, the water in the Earth's mantle is self-fluxing. Water when present in small amounts acts as a trace element and does not affect the total amount of melting or the fluidity of the solid mantle. When present in greater amounts, water increases the amount of melting at given conditions and makes the mantle more fluid. Island arc magma forms when water from the subducted slabs lowers the melting temperature in the overlying mantle wedge (Stolper and Newman, 1994). The preferred amount of mantle water tends to that for transition from trace to major element behavior.

The accretion of water to the earliest Earth is not well understood, but a reasonable mixture of accreting material brings in 20 to 40 oceans. Of that, present mantle water and ferric iron produced from ferrous iron account for around an ocean. Oxidation of the iron metal associated with Pt-group elements in the mantle to ferrous iron consumed another ocean. The fate of the remaining water involves loss of H_2 into the core and loss of H_2 to space (Fukai and Suzuki, 1986). There is enough ferrous iron in the mantle to consume a few oceans.

Other Earth-sized planets need not have the right amount of water to have the familiar oceans and continents. The balance results from internal processes that limit the amount of water in the mantle and violent random processes during accretion that set the total mantle plus surface inventory. The tuning of erosion and tectonics produces the familiar ebb and flow of the sea over continental platforms, which has greatly influenced the evolution of life. A less obvious but more profound effect on complex life is that the right amount of water exists to cover the reducing rocks of the ridge axis but not to cover continental granites, which are the sources of clay in shale. Without a burial ground in shale, organic carbon would have reacted with O_2 and O_2 would not have accumulated in the atmosphere.

Coupled parameterized models for water, oxygen, CO_2 , and other volatile species will be useful for seeing how hypotheses relate to the early Earth and to other planets. The influence of planet size on tectonics can be included by explicitly modeling thermal history and having the rate of tectonics depend on the interior temperature of the planet. The effect of pressure (and hence planetary gravity) on melting is included easily. Again planets with limited planet-wide surface water are simplifications of Earth models.

The Imprint Of Life On The Observable Environment

A non-Earth-centric approach to identifying biosignatures is to consider a fundamental feature that is common to all life. For the purposes of this proposed investigation, the relevant feature of life is that it consumes energy and produces disequilibrium products. In particular, life will consume and add volatile species to and from the planetary environment. The manifest evidence of either process may be detectable in the atmosphere of a planet and serve as a signature of an inhabited planet. Therefore, a second approach we will adopt to model the environmental implications of the presence of life, will be to simulate consumption and emission of gases by various biological mechanisms at appropriate stages in the computed planetary evolution sequence. We will then simulate the fate of biologically emitted gases in the atmospheric-chemical system, including both homogenous gas-phase and heterogeneous processes.

Very few organisms exist that do not consume and/or produce copious quantities of gases, many of which would not be found, even in small quantities, without the catalytic activities of life. Alternatively, the biosphere may result in steady state levels of gases which individually might exist in abiotic atmospheres, but should otherwise not be found together at the observed levels.

Should our search of extrasolar planetary atmospheres encounter evidence of life, that evidence will most likely be the gaseous products of microorganisms. Our biosphere was exclusively microbial for over 80 percent of its history (Schopf and Klein, 1992) and, even today, microbes strongly influence atmospheric composition. Life's greatest environmental impact arises from its capacity for harvesting energy and creating organic matter. Microorganisms catalyze reactions between C, S and transition metal species at temperatures where such reactions can be very slow in the absence of life (e.g., S redox reactions, Des Marais 1996). Sunlight harvested by photosynthesis has created enormous energy repositories in the form of coexisting reservoirs of reduced, organic C and S stored in Earth's crust, and highly oxidized species (oxygen, sulfate and ferric iron) stored in the crust, oceans and atmosphere (Garrels and Perry, 1974).

Ecological processes determine life's distribution and survival and therefore determine our ability to detect life (Des Marais et al., 1998). The evolution and survival of the early biosphere depended upon the efficient coordination of resources and processes among

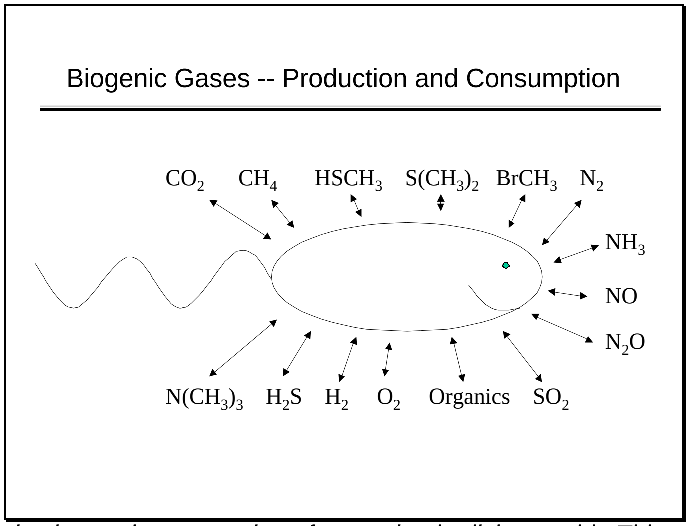


Figure C.3.5.2. Production and consumption of gases by the living world. This cartoon represents some of the known reactions that occur by living organisms with regard to gas production and consumption. All the gases shown are both consumed and produced by some living organisms on Earth, and many are key to the existence of certain groups of organisms. (see Nealson, 1997; Nealson and Conrad, 1999).

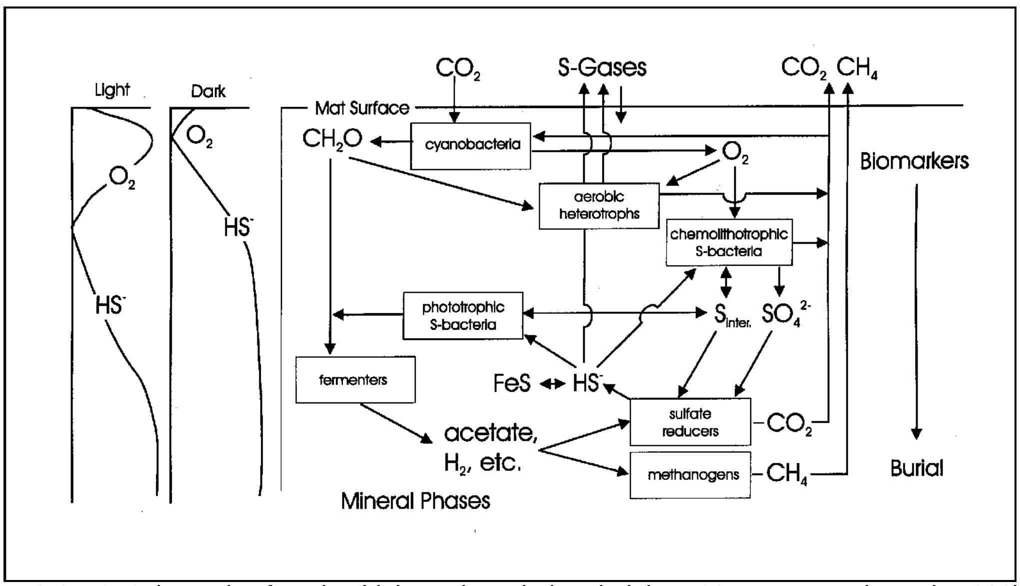


Figure C.3.5.3 Schematic of a microbial mat (Fenchel and Finlay 1995, Des Marais et al., 1998). Boxes denote functional groups of microorganisms, and arrows denote flows of chemical species into or out of microorganisms. S_{inter} indicates S in intermediate oxidation states.

diverse microbial populations. Microbial mats offer an example of such coordination (Fig. C.3.5.3), and they are particularly important because they are the oldest-known ecosystems, as evidenced by their 3.4+ billion-year fossil record. Photosynthetic microbial mats are key because, today, sunlight powers more than 99 percent of global primary productivity (Des Marais 1997; 2000a). For most of Earth's history, photosynthetic ecosystems have affected the atmosphere profoundly and have created the most pervasive fossils. Therefore, extraterrestrial surface-dwelling biospheres that derive energy principally from starlight will be most amenable to astronomical detection (Des Marais, 1999).

While photosynthetic bacteria dominate microbial mats numerically and in terms of productivity, many aspects of the system's emergent behavior may ultimately depend on the associated nonphotosynthetic, including anaerobic, microbial populations (Figure C.3.5.3). The anaerobic zone of the mat represents the ultimate biological filter on chemical, isotopic, and geologic biomarkers passing into the fossil record. Transformation of photosynthetic productivity by anaerobic bacteria may contribute diagnostic "biosignature" gases that could represent search targets for remote spectroscopic life detection efforts. To understand the overall structure and function of mat communities, it is thus critical to determine the nature and extent of interaction between phototrophic and anaerobic microorganisms.

The broadest approach to defining life's role in planetary atmospheres recognizes that planets, environments and biospheres evolve and change (Des Marais, 1999). For example, a tectonically more active early Earth hosted a biosphere that accommodated elevated temperatures (at least locally), was potentially non-photosynthetic, and coexisted with a mildly reducing, CO_2-rich and O_2-poor atmosphere (Veizer, 1994). Microorganisms acquired energy by consuming H_2 and sulfide and producing a broad array of reduced C and S gases, most notably CH_4. Diverse types of bacterial photosynthesis developed that indeed enhanced global productivity but could not yet split the water molecule to produce O_2 (Xiaong et al., 2000). Later, but still prior to 2.7 billion years ago, oxygenic photosynthesis developed (Schopf and Packer, 1987; Des Marais, 2000a). In a planet's evolutionary track, it is possible that the nature of biogenic gas emission will be indistinguishable from the background atmosphere.

We can expect to encounter distant biospheres that represent various stages of evolution and that coexist with atmospheric compositions ranging from reducing to oxidizing. Accordingly, we must be prepared to interpret a broad variety of atmospheres, all potentially containing signatures of life. Apart from what the discussion in Task 3 regarding evidence for the composition of the paleoearth atmosphere in the geological record, remarkably little is known about the composition of our own earlier atmosphere, particularly prior to the rise of O_2 levels some 2.0 to 2.2 billion years ago (Kasting, 1993). Thus, field and laboratory observations are being conducted to examine the relationships between the structure and function of microbial ecosystems and their gaseous products. Ecosystems that are analogs of our ancient biosphere (e.g., based upon chemosynthesis and various types of photosynthesis, thermophilic and subsurface communities, etc.) are, or will soon be, studied. Because key environmental parameters such as temperature, seawater composition, and levels of H_2, CO_2 and O_2 varied during planetary evolution, their consequences for microbial ecosystems are being explored (Des Marais, 2000a, 2000b). Studies of a number of sites that mimic key attributes of Earth's early environment focus upon evolutionary adaptations to long-term changes in the global conditions (Des Marais et al., 1998). These include marine platform settings (carbonate-depositing; hypersaline) similar to those that nurtured ancient stromatolites, and also thermal springs in Yellowstone National Park that resemble analogous ancient thermal habitats (Ames Group). To the extent that rocky planets experience parallel evolutionary trajectories (Des Marais, 1999), this work is also relevant to studies of extrasolar habitable environments.

We propose to integrate a fully parameterized biology component into the IPM. Biological processes directly affect the atmosphere via fluxes of biogenic and bioavailable gases. In turn, local and global fluxes of biogenic gases are affected by changes in the physico-chemical characteristics of the local and global environment. In particular, gas fluxes change in response to changes in length of day, solar insolation, temperature, wind stress, atmospheric composition, rainfall and nutrient availability. At present, data on how particular environmental conditions affect biogenic gas fluxes are relatively sparse, though ongoing research is rapidly changing this situation. We will parameterize the response of the biosphere to changes in these variables at various length- and time-scales using whatever data are available from studies such as those described above. As data are gathered regarding fluxes in and out of microbial mats, the mixed layer of the ocean, soils and other environments, these parameterizations will be improved accordingly. On a global scale these parameterizations will depend in part on assumptions about the fraction of the biosphere in each of the various ecological niches mentioned, which will in turn depend on the configuration of continents and on climate. By scaling up to global fluxes from local experiments and analyses given an assumed continental configuration and climate state, we can investigate how biogenic gas fluxes affect the composition of the atmosphere. In turn, the consequent changes in composition will affect all the relevant parameters and so forth from time step to time step in the model. With a better and better parameterized model we will become increasingly good at estimating the true global impact of life on the atmosphere of Earth, throughout its history, and on the atmospheres of any postulated extrasolar planet.

Time-Dependent Planetary Evolution Scenarios

Like the Abiotic Planet Model, the Inhabited Planet Model will produce time-varying planetary evolution sequences. The processes related to life will be treated as a function of the time-varying planetary context.

C.3.5.2.RESEARCH TASKS

The Inhabited Planet Model is a tool for investigating the influence of life on an environment, and the detectability of that influence using astronomical techniques. Model runs will focus on stellar/planetary combinations that were determined in Task 4 to provide a habitable environment. For each IPM output, a globally-averaged synthetic spectrum will be produced and comparison between these spectra and corresponding abiotic planet spectra will be used to investigate the relationship between life and unique, detectable spectral features. This study will allow us to identify new potential biosignatures, initially for different types of carbon-based life, but with the potential to expand to other forms of life as parameterizations for these forms become available.

We will also use the IPM to address the extent to which the presence of life sustains a habitable environment, and results in a widening of the Continuously Habitable Zone beyond previous estimates. We will also use the IPM to address and explore potential mechanisms for the rise of oxygen on our own planet.

In the following sections, we briefly expand upon the latter two research tasks.

Life And Climate Stability

Climate modelers have long relied on the Walker feedback mechanism to explain the long-term stability of Earth's climate and its operation remains the most plausible explanation for why the Earth's climate has remained relatively stable over the last 2 billion years. However, the empirical constraints on CO_2 levels suggest that there was not enough CO_2 in the atmosphere prior to ca. 2.2 Ga to support this sort of mechanism and that another greenhouse gas, e.g. CH_4 may have played a critical role in warming the Earth (Rye et al., 1995). There is no well-established or widely accepted mechanism to explain how Earth's climate would have been stable for hundreds of millions of years under a CH_4-CO_2-H_2O greenhouse. Nor do we understand why this system failed and shortly thereafter O_2 rose dramatically, essentially forcing the system to rely on CO_2. The model we will develop will allow us to test a series of possible explanations for both of these geological events.

A detailed understanding of the ways that climate and atmospheric chemistry affect life *and* vice versa are essential to any explanation of climate stability in which a biogenic gas plays a key role. As an example of the integrated nature of the system we are attempting to model and the possible complexity of the cycles that may drive it, we describe the following experiment, which we will test with the IPM.

For an Earth atmosphere with 20 µatm CH_4, < 2000µatm CO_2 as well as H_2O (with CH_4 largely biogenic in origin) we ask whether the following feedback loop could maintain a stable climate for hundreds of millions of years. Let CH_4 accumulate until CH_4/CO_2 equals 1. A UV absorbing haze will form. Biogenic NH_3 will begin to accumulate in the atmosphere. At high enough NH_3 levels, rain pH will increase above 7. Weathering essentially will cease. Phosphate delivery to the ocean will shut down. Over a time scale of a few thousand to tens of thousands of years, primary productivity will drop dramatically. Biogenic methane production will eventually follow. As CH_4 falls and CO_2 accumulates CH_4/CO_2 goes to < 1. The UV screen and the NH_3 will disappear. Rain pH will fall and weathering will restart. CO_2 levels will also begin to fall. Primary productivity recovers. CH_4 begins to accumulate again. And so forth. Many questions arise immediately. Could long-term outgassing provide enough H_2 to reduce enough CO_2? How long would it take before loss of H_2 to space shut down the system? Would a UV screen really form? How would the NH_3 abundance really respond to changes in UV flux, when one included the effects of changes in nutrient availability? How would CH_4 production be coupled to global primary productivity in such a world? etc. Such a scenario can only be fully tested by a fully coupled model, though of course, if any point in the loop simply cannot work the whole loop would have to be modified or discarded. The point is that, when biogenic gases play a key role in postulated climates, we need not only to account for the radiative effects of the gases but also keep track of the impact of a variety of changes, including rain chemistry, weathering rates and consequent nutrient availability, cloud and/or aerosol microphysics and so forth. This scenario is illustrative of the sorts of interactions that could be of importance in understanding Earth's present and past as well as the atmospheric chemistry of any postulated inhabited extrasolar planet. Understanding these interactions and modeling their consequences will allow us to address what Earth's atmospheric spectrum may have looked like from space throughout Earth history and what other planets with non-Earth like histories might have looked like as well.

The Rise Of Oxygen

An understanding of the rise of oxygen in Earth's early history provides a basis for simulating the rise of oxygen in other inhabited worlds, and understanding what these planets would look like spectroscopically during various stages in their evolutionary history. Two of the current ideas on why the Earth seems to have had little free O_2 before about 2.3 Ga are best supported by available evidence.

(1) O_2 is controlled by the disproportionation of a more or less fixed CO_2 inventory, and the extent of disproportionation increases over time (i.e. the reservoir of buried reduced carbon increases with time). Carbon isotope data provide support for the hypothesis that a massive pulse of reduced carbon burial accompanied the first rise of O_2 (Karhu and Holland, 1996). Increasing disproportionation of CO_2 could be driven by geological or biological changes. A geological change might consist of continents growing larger and less subject to metamorphism and weathering (processes that liberate buried carbon). This is probably the leading hypothesis, and one that one can hope to model. A related geological argument is based on the observation that carbon is buried in clays. Clays derived from basalt contain a great deal of ferrous iron, which can easily consume the oxygen derived by burying reduced carbon. Clays derived from granite contain little ferrous iron, so when reduced carbon is buried, free O_2 is left behind. A progressive change from basaltic to granitic weathering is documented in the strontium isotope record, with the transition occurring towards the end of the Archean (Godderis and Veizer, 2000). Both geologically-based hypotheses are tied to the origin of continents and therefore are potentially generalizable to other terrestrial planets. A biological (or Gaian) argument would be the progressive development of better pumps to dynamically separate the C from the O_2. In effect Gaia gets ever better at pushing the C down or pushing the O_2 up. Again, if the driving force is biological, it provides a challenging situation to model.

(2) Hydrogen escape from an early reduced atmosphere changes the redox state of the Earth near the surface (Catling et al 2000). Circumstantial evidence in favor of biogenically-supported methane-rich ancient atmospheres on Earth provides intriguing context. An effective methane greenhouse would make secular oxidation inevitable. In this hypothesis all accessible reduced reservoirs are titrated, and eventually become poorer at removing photosynthetically produced O_2 than the oxidized reservoirs are at removing CH_4. (One key photochemical issue is the degree to which CH_4 and O_2 can coexist.) This differs from pure disproportionation of CO_2 because it posits that the oxidation state of the crust determines the lifetime of the oxidant generated by disproportionation. This process can be heuristically generalized to other terrestrial planets by calibrating the titratable reservoirs to Earth.

C.3.5.3PRODUCTS AND SIGNIFICANCE

This task will produce a comprehensive suite of physically, radiatively, chemically and biologically self-consistent atmospheres for a range of possible extrasolar terrestrial planets both with and without different forms of dominant life.

The synthetic spectra generated from these atmospheres will be used to define new potential biosignatures using astronomical instrumentation, and will be offered to the community as a reference source for the design of instruments for planet detection and characterization.

We will also provide specific recommendations and guidelines derived from these spectra for the best spectral range, spectral resolution and signal to noise ration required to detect these biosignatures, and test for their detectability using a variety of likely instrument and telescope designs.

The IPM, and the entire VPL, will be a tool for use by the science team and a forum for collaborations between the science team and NAI member scientists and members of the broader astrobiology community. The IPM will be programmed in a modular fashion to allow easy exploration of alternative formulations of processes integrated in the IPM simulation of a planet.

RELEVANCE TO NASA INTERESTS

The proposed work will expand the scope of existing research being undertaken in the NASA Astrobiology program. It will provide a comprehensive, systematic study of capabilities for the remote-sensing detection of extrasolar life, to augment existing NAI focus on detection of life within our own Solar System.

In so doing, this research program will provide practical, timely, and much-needed recommendations and guidelines for development of future NASA missions that seek to detect and characterize extrasolar terrestrial planets, such as TPF and its second generation follow-on, Life Finder. This work will not only drive the design and survey strategies of these missions, it will also provide an initial solid theoretical basis for the interpretation of the results of these missions. The following table maps the VPL Products and Tasks into the NAI Goals and objectives.

The proposed work, including the modeling tools and spectroscopic results, will also be valuable for research in many other NASA research programs including Planetary Astronomy, Planetary Atmospheres, Sun-Earth Connection, and the Origins program. These tools and results may also be of use to the design of future Discovery proposals that seek to discover or characterize extrasolar planets

NAI ROADMAP GOALS AND OBJECTIVES	**VPL PRODUCT**	**TASK**
Does Life Exist Elsewhere in the Universe? Goal 7 Determine How to Recognize the Signature of Life on Other Worlds. To understand remotely sensed information from planets circling other stars, we should develop a catalog of possible signatures of life.	Development of Spectral Catalog of Habitable, Uninhabited and Inhabited Planets	Tasks 1-5
Does Life Exist Elsewhere in the Universe? Goal 7 Essential to learn to identify the chemical signatures of life on a distant world through remote sensing of its atmosphere or surface. For the previous several billion years during which Earth had life, the atmospheric and surface signatures are not fully understood. In exploring other worlds, it is critical that we generalize the process of coevolution of planet and life.	Better Understanding of the Spectral Appearance of Earth's Paleoatmospheres	Tasks 2-5
Extrasolar Biomarkers Objective 13 Define an array of astronomically detectable spectroscopic features that indicate habitable conditions and/or the presence of life on an extrasolar planet. We must develop the database for interpreting those spectra, both for evidence of habitable conditions (e.g., the presence of liquid water) and for evidence of life. Aspects of the strategy include developing appropriate observational approaches that optimize sensitivity and spectral and spatial resolution, creating models of atmospheric chemistry and its evolution, and achieving an understanding of the factors that control the composition of biological gas emissions to the atmosphere. We must develop the ability to discriminate between those environmental conditions and gas compositions that indicate a geologically active but "lifeless" planet, versus those conditions and compositions that compel a biological interpretation. The requirements for detecting extrasolar biospheres in association with a range of atmospheric compositions will be key drivers behind the designs of interferometric telescopes that will obtain spectra of extrasolar planets. The astrobiology research program therefore must contribute substantially to the optimization of those designs. The program must lead the continuing search for novel methods to detect remote biospheres spectroscopically. Provide recommendations for instrument capabilities and search strategies to optimize designs of future instruments that will obtain spectra of extrasolar planets.	Provide atmospheric compositions of habitable planets that lack biospheres. Determination of potential false positives Emission of biogenic gases as a function of planetary environment Develop global models for the composition of Earth's early reduced atmosphere Calculate synthetic spectra of a range of plausible extrasolar planetary atmospheres, both with and without free O_2. Identify a menu of biologically-produced volatile atmospheric species. The spectral signatures of plausible extrasolar planetary surfaces both with and without life that might be detected remotely.	Tasks 3-5 Task 4 Task 5 Tasks 3-5 Tasks 2-5 Task 5 Tasks 1-5
Effects of Climate and Geology on Habitability Objective 12 Define an array of astronomically detectable spectroscopic features that indicate habitable conditions and/or the presence of life on an extrasolar planet.	Best available estimates of the habitable zone using physically, chemically and radiatively self-consistent atmospheres with realistic clouds. Better models for how hydrogen escapes Realistic paleoatmospheres for early Earth Effects of geology on planetary atmospheric composition and effects on habitability Effects of biology on planetary atmospheric composition and the limits of the habitable zone.	Task 3 Task 4 Task 2-5 Task 3-4 Task 5

C.5 WORK PLAN AND SCHEDULE

TableC.5.1 shows the five major Tasks, the sub-task components and the members of our team working each component.

Table C.5.1
Allocation of Personnel to the Five Major Tasks and sub-task components
Leads responsible for each overall Task, and then for each subtask are indicated with an L.

	Meadows	Allen	Brown	Cohen	Crisp	Fijany	Huntress	Kasting	Nealson	Richardson	Rye	Sleep	StorrieLombardi	Velusamy	Yung	Zahnle
Task One Lead Scientist - Meadows																
Conversion of SMART and LBLABC to ultracomputing					♦	♦							L			
SMART global grid simulations for Earth	L		♦		♦											
Validation of SMART spectra with Earth data	♦				L											
Experiments to determine sensitivity to known changes in trace gas abundance, surface albedo, cloud distribution, phase angles, viewing geometries	L				♦											
Astronomical instrument simulator assessments of sensitivity to these parameters	L													♦		
Identification of potential biosignatures from the atmosphere and surface	L				♦											
Mars, Venus and Titan global grid simulations and validation.	♦				L											
Task Two Lead Scientist - Meadows																
Completion of SMARTMOD	L															
Upgrade SMARTMOD to ultracomputing	♦				♦	♦							L			
Validation of SMARTMOD	♦				L											
Task Three Lead Scientist - Meadows																
Incorporate 1-D chemical model into SMARTMOD	L	♦			♦										♦	
Upgrade combined model to ultracomputing		♦			♦	♦							L			
Determination of the Habitable Zone for these atmospheres	L		♦	♦	♦			♦								♦
Synthetic spectra of Earth paleoatmospheres	L		♦		♦		♦	♦			♦					
Synthetic spectra for modern and early Earth around other stars	L		♦	♦	♦		♦	♦			♦					
Run tests for the detectability of varying amounts of the currently accepted biosignatures in a range of plausible habitable atmospheres around stars of different spectral type	L			♦	♦			♦								
Determine the optimum wavelength range and spectral resolution for detection	L				♦											
Run through instrument simulators	♦													L		
Determination of detectability of biosignatures for paleoearth and planets around other stars	L							♦						♦		
Development of statistical tools for analysis of the biosignature catalog	♦												L	♦		
Task Four Lead Scientist - Allen																
Ultracomputing		♦				♦				♦	♦		L			
Escape of gas to space								L		♦						♦
Effects of small bodies entering the atmosphere										♦						L
Land/Ocean/Interior		L					♦	♦			♦	♦			♦	
Determination of false positives	L				♦			♦		♦	♦			♦	♦	
Task Five Lead Scientist - Allen																
Ultracomputing		♦				♦				♦			L			
Biology			♦				♦		L		♦	♦				
Determination of new biosignatures	♦	L			♦			♦	♦	♦	♦					
Spectral catalog for physically, radiatively, chemically and biologically self-consistent atmospheres	L				♦			♦								
Recommendations for instrument parameters, designs and search strategies	L				♦									♦		

C.5.1 SCHEDULE OF RESEARCH TASKS

To implement the tasks outlined in Section C.5, we will begin work on Tasks 1, 4 and 5 in the first year of this effort. Task 1 will determine sensitivity to environmental characteristics in the globally averaged synthetic spectra of terrestrial planets using a radiative transfer model, and will provide the first step for development of the subsequent modeling tools. This task is scheduled for completion 6 months after the start of this effort (the receipt of funding). The design and development of models for the geological, exospheric and biological sources and sinks of volatiles will be done in Tasks 4 and 5 and will start simultaneously with Task 1, continuing for the next 4-5 years. Task 2, the next step in the development of the modeling tools, will validate a climate model and the 1D globally averaged approach used in our modeling. This task starts immediately after completion of Task 1 and will take 9 months to complete. Task 3, integration of a chemical model with the climate model validated in Task 2, completes the mechanistic core of the planet models to be developed in Tasks 4 and 5 and finishes in the 2nd quarter of CY03. Work in the final two years of this effort will concentrate on integration of the ongoing parameterization of geological and exospheric sources and sinks of volatiles into the coupled radiative-climate-chemical model to produce the Abiotic Planet Model at the end of Task 4. Integration of the biological model components into the Abiotic Planet Model will produce the Inhabited Planet Model. At all stages of model development, scientific results, synthetic spectra, and recommendation for instrument parameters will be produced.

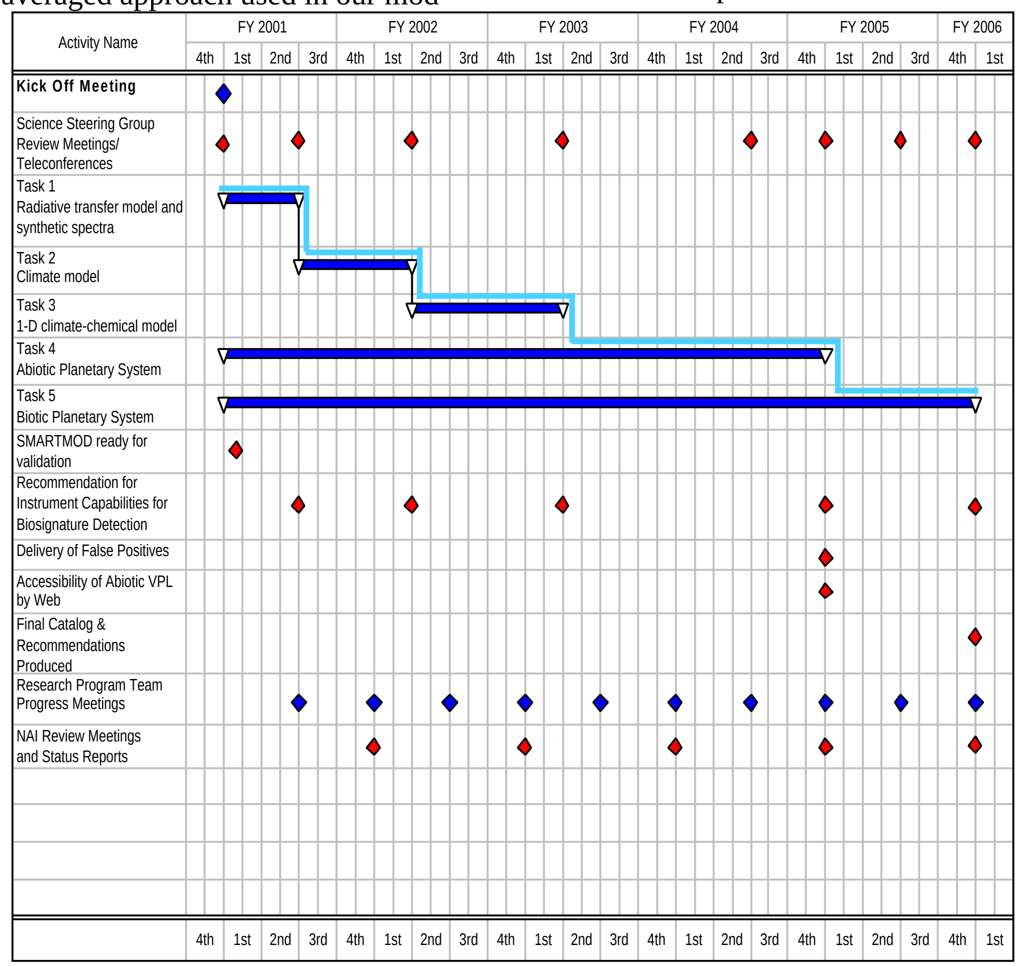


Figure C.5.1 Astronomical Detection of Biosignatures key tasks and milestone schedule

C.6 MANAGEMENT PLAN

This research program is a cooperative effort consisting of a 17 member multidisciplinary team that leverages the resources and knowledge from 7 academic and research institutions. The majority of the computational research will be accomplished at JPL/Caltech, although all institutions will provide investigators' scientific expertise. Coordination and integration of the efforts of the research team members, in a timely manner, is the focus of this management activity. The framework in which this will be accomplished will be addressed in three areas: Organization and Decision Making; Schedule (discussion in Section C.5.1); and Tracking, Review and Reporting.

C.6.1 ORGANIZATION AND DECISION MAKING

The organizational structure of the research program is shown in Figure C.6.1 (Org Chart). The PI, Dr. Victoria Meadows, is accountable to NAI for the implementation, outcome, and scientific integrity of the research and its products. The overall direction is the responsibility of the PI, however, when unavailable the PI will temporarily delegate management authority to a member of the Science Steering Group.

The research efforts of the program will be accomplished within five major task groups, each with a Lead assigned. Issues that are not resolved between or within the task groups will be resolved by the PI, who is the final arbiter. In addition to other responsibilities discussed (Section C.6.1.2), a Science Steering Group, consisting of lead scientists from this effort, will advise the PI and provide additional assurance of the integrity and focus of achieving the research objectives on schedule. The organizational structure also shows the EPO effort and the administrative support, which will provided by the PI's home institution. The EPO effort will be managed in manner similar to the research tasks (Section C.6.1.1).

C6.1.1. TASK GROUPS

The individual research tasks performed under the proposed effort are coordinated within task groups, maintaining the focus of the work on the program’s objectives. Each task group has a leader whose responsibility is to maintain this focus and coordinate the overall work with other task groups and with the NAI. Each task group has subtask components and each component has been assigned a lead scientist, (Table C.5.1).

C.6.1.2 SCIENCE STEERING GROUP

The Science Steering Group will assist Dr. Meadows in performing her many responsibilities as Principal Investigator. The SSG consists of the following senior personnel: Allen, Crisp, Huntress, Kasting, Nealson and Sleep and has the primary function of integrating the work carried out in all the task groups.

The specific functions of the SSG will be to assist Dr. Meadows in:

The review and assessment of overall progress towards the goals of the research program

The coordination of tasks within the research program

Arranging and conducting general co-investigator meetings

The promotion and implementation of interactions with the NAI

Facilitation of communication among the team members and with the NAI

Development and implementation of a policy for the publication of scientific results from tasks performed by the team members

Assuring all reporting requirements are met

In addition, the SSG will assume such responsibilities as may be delegated by the Principal Investigator.

The SSG will interact by teleconference and will meet to carry out its responsibilities.

C6.1.3. ADMINISTRATIVE SUPPORT

Dr. Meadows will draw upon JPL’s Earth and Space Sciences Division for administrative support. The Earth and Space Sciences Division maintains Offices of Scientific Administration (OSA) that support routine administrative needs of PI tasks within the division at no direct cost to these tasks. This support includes the handling of procurements, contracts, travel arrangements and account management. Upon the award of the contract, JPL will execute required contracts with participating institutions for non-government funded Co-I support.

C.6.2 TRACKING AND REPORTING

The PI will establish and implement as simplified financial tracking and reporting system. This will be used to assure that the research planned is accomplished within the allocated funding and schedule profile. Status of these activities will be assessed quarterly and be available for NASA review and will be rolled up into the final report.

We will provide annual and final reports as specified in Section A (revised October 1997) of the NASA Grant and Cooperative Agreement Handbook. Annual progress reports provided by each of the task leaders will be integrated by the PI and used as the technical basis for these reports. These elements will be supplemented with financial and schedule data accumulated over the annual reporting period as discussed above.

C.6.3 RESEARCH REVIEWS

A Co-Investigators Meeting will be held biannually to facilitate scientific collaborations among the members of this research program and to assure progress towards a common goal. All Co-Is and post-docs will be invited to this meeting and all interested NAI members. The task leaders will report annual progress for peer review at this meeting. Our research program will also support NAI's annual integration workshop and we will participate in the preparation of workshop reports. All research products will be documented in the open literature and available for the NAI/scientific community for review.

C6.3.1. NEXT GENERATION INTERNET

The Next Generation Internet (NGI) will be used heavily to manage the research activities outlined in this proposal. Since all co-investigators are at or near institutions already having a NAI-supplied videoconferencing area, most of the monthly science advisory group meetings and the quarterly co-investigator meetings will be held as videoconferences. In addition, we will utilize extensively collaborative software that runs on desktop computers to allow simultaneous visualization and analysis of model results by multiple members of the science team sitting at their home institutions. There are several applications programmed in Java that would facilitate such interactions because a common program could operate under a variety of host computer operating systems. The Internet will be used to allow members of the science team from their home institutions to execute model runs on the JPL supercomputers and retrieve results.

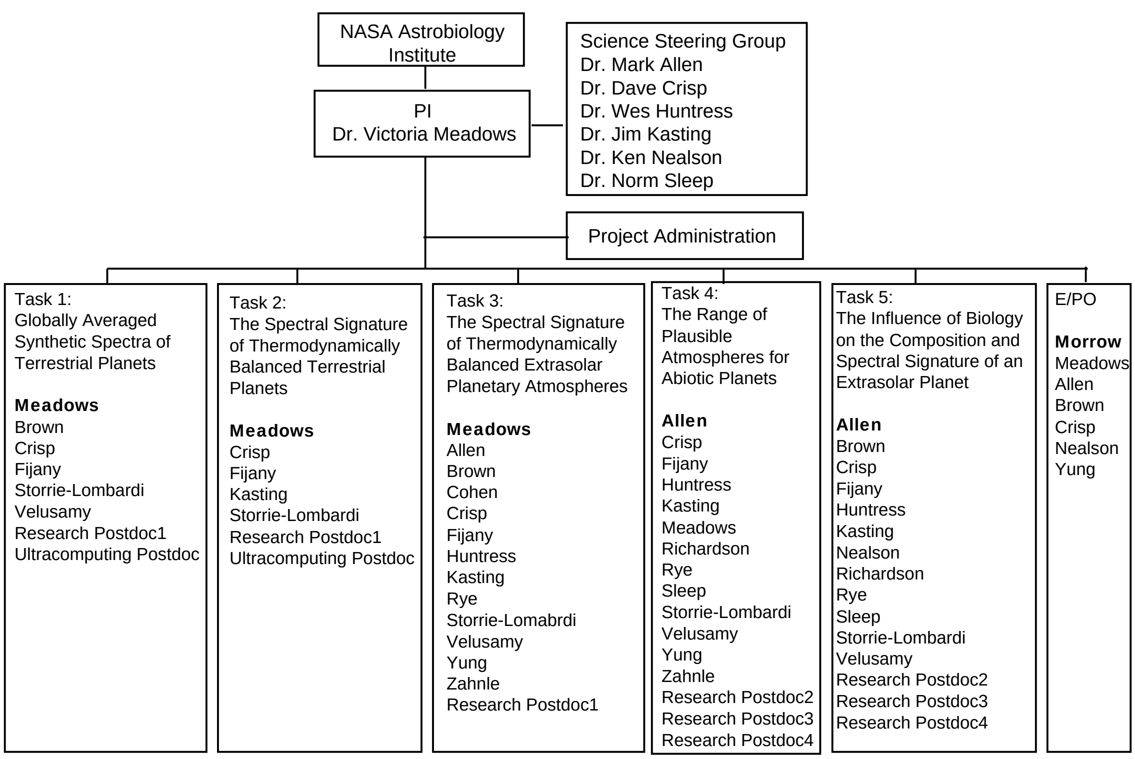


Figure C.6..1 Organization Chart

C.7 STATEMENT OF CONTRIBUTIONS BY PI & CO-IS

Dr. Victoria S. Meadows, (JPL) is the Principal Investigator and is accountable to NASA for the overall research program. Dr. Meadows has had extensive experience on mission design and development work and understands the importance of schedule and delivery and integration of multiple components. She is committed to working in a team environment to accomplish a common goal.

Dr. Meadows will assure that the scientific goals of the program are met on schedule, and the members facilitate the overall objectives of the NAI. Dr. Meadows will be supported in this role by the Scientific Steering Group , whose members will be: Allen, Crisp, Huntress, Kasting, Nealson and Sleep.

C.7.1 THE MULTIDISCIPLINARY TEAM

This multidisciplinary team is composed of 17 scientists from Caltech, JPL, Penn State, Berkeley, Ames, Stanford, Carnegie and Univ. of Colorado, all who are experts in the respective fields. The majority of the research program activities occur at JPL/Caltech. The scientists include not only atmospheric chemists, physicists, and radiative transfer specialists, but astronomical observers with experience in ground-based and space-based observing, and spacecraft mission design and support. This team understands both the atmospheres of terrestrial planets, and the realities and limitations of astronomical observing.

Dr. Vikki Meadows (JPL), the team leader exemplifies the multidisciplinary qualities of JPL/Caltech by being trained both as an observational astrophysicist and as a planetary atmospheric scientist. Her work has focused on remote-sensing retrieval of gases and aerosol properties from infrared observations of planetary atmospheres. She will lead the development of a suite of radiative-transfer tools to characterize the detectability of astronomical biosignatures and make recommendations to drive future instrument designs. Expertise in modeling atmospheric chemistry and photochemistry for the global model will be provided by Prof. Yuk Yung (Caltech), a world leader in this field, and by Dr. Mark Allen (Caltech/JPL) will serve as the lead for the Planetary Models experience with incorporating disparate modules into a global planetary model will be provided by Dr. Mark Richardson (Caltech). The radiative-transfer components that will be part of the global model, as well as the means to synthesize spectra of extrasolar planet atmospheres will be provided, updated and maintained by Dr. David Crisp, who is a world leader in state-of-the-art, highly accurate, spectrum-resolving radiative transfer models. Up-to- date and custom spectroscopic molecular line parameters will be provided as input to the radiative transfer and climate models by Dr. Linda Brown (JPL). The best available stellar spectral energy distributions will be collated for us by Dr. Martin Cohen (UC- Berkeley) as input to the radiative transfer, chemistry and climate components of the model.

Caltech/JPL will provide the central expertise in atmospheric science and modeling, we have also recruited additional experts from around the nation to provide us with input on the many processes that have to be considered in creating a global model. Information on hydrogen escape processes, and proven expertise in coupled chemical and thermal radiative convective equilibrium models will be provided by Astrobiologist, Prof. Jim Kasting (Penn. State). Geological sources and sinks of volatiles and the impact of plate tectonics on planetary climate and atmosphere will be provided by Prof. Norm Sleep (Stanford). Available information on plausible abiotic and biotic paleoatmospheres, and the chemistry and products of subsurface processes, including hydrothermal vents, will be brokered by Wes Huntress in collaboration with the Carnegie Geophysical Lab. The impact of biological processes on planetary atmospheres (and in particular the likely biogenic gases produced by different forms of life) will be collated and provided by Prof. Ken Nealson (Caltech/JPL) and Dr. David DesMarais (Ames) and their Astrobiology research teams. Dr. Rob Rye will provide expertise in paleoatmosphere and biogeochemical cycles. The effects of impacts on the chemistry of a planet, and detailed models of hydrogen escape will be provided by Dr. Kevin Zahnle (NASA Ames). Detailed understanding and modeling of the detectability of planetary biosignatures in the context of their planetary system with realistic astronomical tools will be provided by Dr. Thangasamy Velusamy (JPL).

This large and innovative modeling effort will clearly require a great deal of computing performance. Dr. Michael Storrie-Lombardi is an astrobiologist in the JPL ultra computing group. He will act as our liaison through Dr. Amir Fijany, as we work with them to adapt the planetary model to run on JPL's suite of high performance machines.

C.7.2 COLLABORATION WITH OTHER INSTITUTIONS

In addition to the personnel who are identified explicitly on this proposal, we have set up collaborative agreements with the Carnegie Geophysical Laboratory and with other members of the NAI based at Carnegie and at Ames. Huntress will act as broker for collaborative work with CGL and the Carnegie Astrobiology Group, and Nealson will act as interface and broker for work being done by Dave Des-Marais' Astrobiology Group at NASA Ames. Each of these collaborative agreements allows us a "window" into the research being done at these institutions, and will provide important constraints and input to several of our proposed models, using instrumentation and facilities that would not be available at JPL.

C7.2.1. GL COLLABORATION

The Geophysical Laboratory conducts state-of-the-art laboratory research in fundamental geochemical and biochemical processes relevant to understanding the current and early state of planets. The following listing includes some of the processes being studied at GL (with their relevance to this proposal given in parentheses).

1. Elemental, isotopic and chemical analysis of extrasolar materials (exogenic source materials) and geologic samples (biogenic processing of geomaterials).

2. Laboratory and theoretical work on melt processes and rock-volatile chemical equilibrium (coupling of interior chemistry with the atmosphere).

3. High-pressure chemistry (internal source and evolutionary processing of planetary volatiles).

4. Hydrothermal vent chemistry (pre-biotic chemistry and early biochemistry, evolution and cycling of planetary volatiles).

5. Mechanisms of biological metabolism (evolution of energy sources for planetary biology, and evolution of global volatiles).

6. Biological diagenesis (cycling of biological elements and biogenic volatiles).

The GL is currently one of the founding elements of NASA's Astrobiology Institute and is carrying out fundamental and significant work on hydrothermal systems and the origin of life. Recent laboratory work has shown the synthesis of simple biochemical molecules important as initiators in ubiquitous biochemical cycles by the interaction of reduced carbon (carbon monoxide) with venting iron sulfides at elevated pressures and temperature as in hydrothermal vents. The development of life during a vigorous phase of hydrothermal activity on a young planet will have a significant effect on trace and perhaps major components of the atmosphere. These processes will consume early inorganic reduced gases in the atmosphere and convert them into more complex organic components inevitably altering the oxidation state and trace volatile inventory in the atmosphere. These altered components and their relationship may provide an atmospheric signal for microbial biology.

The questions being pursued at GL in hydrothermal geochemistry relevant to the proposed work include the following. What range of planets develop hydrothermal systems and what are the sources and distribution of volatiles within these systems? To what extent and by what mechanisms do organic compounds form in hydrothermal systems and what is the role of mineral catalysts? What processes of self-organization can occur and what steps lead from non-life to life? The work being proposed here would provide a theoretical modeling construct to quantify the effect of global hydrothermal processes on the atmosphere and provide a context for understanding the external detectability of pre-biological and early biological on young planets.

Dr. Huntress will act as a broker between the Geophysical Laboratory (GL) and the research team to integrate the expertise and facilities at GL with the proposed work on chemical characteristics of planetary atmospheres and surfaces. The laboratory work on chemical processes at GL in hydrothermal vents will be an important contribution to the proposed theoretical modeling work on extrasolar planetary atmospheres. Dr. Huntress will provide the interface to the modeling work in this proposal. To facilitate this collaboration, he will attend the SSG meetings.

C7.2.2. ASTROBIOLOGY AT AMES

The team's biology co-investigators will be in close contact with the NAI Ames team of microbiologists and ecologists to define key life-related processes that influence the state of a planetary atmosphere. The team at NASA Ames is led by Dr. David DesMarais, and is actively involved in data gathering related to biogenic gas production and consumption at a number of sites. They have a number of foci of activity and their data, as well as their models for global fluxes will be of great value to the overall success of our proposed modeling activities. Their considerable efforts and expertise demonstrate the way in which the Astrobiology virtual institute can lead to valuable collaborations in areas of immense importance to the scientific community and to the agency.

The Ames NAI Team's current research in microbial ecology is directly applicable to defining life's contributions to the atmosphere during a planet's history.

Key members of the Ames team include the following: David DesMarais (Ames), team leader, coordinated a 10-year field study of the mat ecosystems at Guerrero Negro, Mexico, and is an authority on the biogeochemical carbon cycle. Brad Bebout (Ames) has conducted extensive biogeochemical analyses of microbial mats. Pieter Visscher (University of Connecticut) has conducted studies in biogeochemistry, mat ecology, and the production and consumption of reduced biogenic gases. Chris Potter (Ames) has constructed several ecosystem models, some of which integrate local biogenic gas emissions into estimates of global fluxes. Robert Chatfield (Ames) has developed multidimensional models for atmospheric chemistry, with specific attention to trace gases. Linda Jahnke (Ames) has extensively studied biomarker compounds and carbon isotope discrimination in bacteria. Tori Hoehler (Ames) is a biogeochemist with extensive experience in anaerobic processes in coastal marine environments.

The Ames team is examining the roles played by ecological processes in the early evolution of our biosphere, as recorded in geologic fossils and in the macromolecules of living cells. (1) It is defining the microbial mat microenvironment, which was an important milieu for early evolution. (2) The team will compare mats in contrasting environments to discern strategies of adaptation and diversification, traits that were key for long-term survival on early Earth. (3) Ongoing studies of budgets of solutes and gases in mats will contribute to better estimates of biogenic gases in Earth's early atmosphere.

In collaboration with the team of Dr. M. Sogin, Marine Biology Laboratory, the Ames team proposed an "Ecogenomics Focus Group" (EFG) within NAI. This project was recently funded, and it will begin to define the relationships between microbial diversity, complex gene expression patterns, and biogeochemical processes that shape planetary environments. In this work, 1) the EFG team will characterize biogeochemical patterns in the microbial mats with special emphasis upon gradient location and shape, 2) the team will employ molecular techniques to develop a quantitative assessment of microbial population structure in this microbial ecosystem, 3) EFG will use DNA microarrays to measure gene expression patterns for genes of known function at different locations in the environment, and 4) the team will explore responses to transient and periodical environmental perturbations imposed by diel cycles. Finally, based upon the results of these empirical measurements, 5) EFG will model feedback loops between microbial gene expression and key biogeochemical processes, including gas production, that influence planetary environments.

The model will be verified with observations and rate data determined in the laboratory and field: namely the production, consumption and flux estimates of volatile C and S compounds made in a variety of microbial mats (gas fluxes: VOSC, CH_4 from hyperaline mats; measurements: DMS, MSH, DMDS, ESH, CH_4 from temperate mats [e.g., Visscher and Taylor, 1994, Visscher et al., 1994, 1996, and other papers]). Data on microbial metabolic rates that produce and consume gases and/or volatile compounds, that are required as input parameters for the model, will be supplemented with results from ongoing studies and mat manipulations by the Ames NAI team. Alternate or successive physical conditions of the earlier-Earth surface environment will be evaluated in simulation trials. These will determine the possible outcome of competition for light and gaseous and mineral substrates in the microbial mat ecosystem, and related effects on predicted bio-emission estimates of O_2 and CO_2 gases and other volatile species. In order to accommodate the implications of the long-term evolution of inhabited worlds, it will be important to compare these simulations with careful manipulations planned by the experimentalists : e.g., exposing mats to environments that represent plausible extrasolar planetary atmospheres, as identified by atmospheric scientists.

C.8 TRAINING PLAN

Our proposed research program will provide many opportunities for training of undergraduates, graduate students, and postdoctoral fellows. The training will provide exposure to many disciplines supporting astrobiology and in methods for multidisciplinary research. Our specific programs in education and training are described in the following sections.

C.8.1 UNDERGRADUATE EDUCATION

There are several undergraduate education avenues that will provide opportunities to participate in astrobiology-related research. These are important parts of our program, as they are one of the major ways in which undergraduates will be attracted to graduate work in the general area of space sciences, and astrobiology in particular.

C.8.1.1 JPL AND CALTECH

Summer Undergraduate Research Fellowship (SURF) and Minority Undergraduate Research Fellowship (MURF) Programs are directed at providing significant research opportunities for students at the undergraduate level. The MURF program is aimed at improving the representation of African-Americans, Hispanics, Native Americans, Puerto Ricans, and Pacific Islanders in science and engineering. The competition is open to undergraduates around the country, and is advertised through the Caltech Homepage. Interns are selected competitively. We will participate in both programs by submitting a short description of the proposed astrobiology research program and its co-investigators, and selecting students for the summer internships.

The biology component of our work has some excellent opportunities for undergraduate training. We expect that students will be particularly interested in combining biological field work funded by other programs with the physical and chemical modeling activities in our research program. A student who is comfortable in translating information from one discipline into an appropriate context for another discipline is the sort of student that we hope to produce as a result of our program.

Dr. Victoria Meadows, the Principal Investigator, has supervised 2 SURF students, 1 for one year and the other for 3 years during the past 3 years. Her students have gone on to graduate student programs in extrasolar planet detection and atmospheric remote-sensing.

The JPL/Caltech team members have collectively supervised 17 SURF students over the past three years.

Dr. Ken Nealson has directed at Harvey Mudd College a special undergraduate program in astrobiology—the Harvey Mudd Clinic Program—in which 5-6 undergraduates are trained per year in a research-intensive program.

The Caltech Division of Geological and Planetary Science (GPS) offers undergraduate courses in astrobiology. Dr. Ken Nealson teaches three different classes. The first is a course in microbial diversity and extremophiles, the second is a course in geobiology, called “Microbes and Minerals”, and the third is a course taught with Professor Yuk Yung, called “Habitable Planets”. This team will augment the existing curriculum by providing coursework highlighting remote-sensing detection of biosignatures and multi-disciplinary studies of the climate, chemistry, and habitability of terrestrial planets. Using the interconnective abilities of the Next Generation Internet (NGI) system, we will endeavor to offer this course in all of the member institutions of this research program, and even in institutions of other members of NAI. We are fully committed to interactions within NAI, and this approach will be a focal point for attracting undergraduates. We will explore the possibility of providing tapes of these lectures, thus building a library of educational materials at the undergraduate level. We will also explore the possibility of using the Internet for course offerings.

C.8.1.2 STANFORD UNIVERSITY

Planetary habitability is presented in both introductory and advanced undergraduate courses.

C8.1.3. CARNEGIE INSTITUTION OF WASHINGTON

CIW science staff teach at universities, and many staff members work in collaboration with university colleagues. These interactions generate opportunities, on an individual basis, for undergraduate research work at CIW. The advantages to the students are the interaction with additional science staff there and access to state-of-the-art research facilities. There are generally 2-3 undergraduates working at any one time.

In addition, there is an active summer intern program for undergraduates that are supported jointly by the National Science Foundation and CIW. About 15 students participate each summer.

C.8.1.4 ALL PARTICIPATING INSTITUTIONS

NASA Planetary Biology Internship (PBI). The PBI program offers outstanding undergraduates (and beginning graduates) the opportunity to spend summers in NASA-related research laboratories. For example, Dr. Nealson had two PBI interns doing interdisciplinary science in his Caltech laboratory. We will add the members of our program to the list of labs that are qualified to accept PBI interns.

The proposed research program will complement the existing activities of NAI members. Also detailed in this proposal are explicit collaborations already planned for the science team to work with the Ames Research Center and Carnegie Institution of Washington NAI members. However, in addition to actively participating in NAI workshops, science meetings, and committee deliberations, the science team will provide access to the research models developed in the proposed effort via the Internet and the Web for NAI member scientists and others in the larger Astrobiology community to explore ideas about the evolution of the Earth and other terrestrial planets. Many astrobiologists have ideas about how some portion of a planet works. Our flexible models will provide the opportunity to those with ideas to explore the implications of their hypotheses in the context of the “virtual” planet simulations. Lastly, results of science team activities will be communicated to other members of the NAI using NGI via videoconferencing and Web postings.

C.8.2 GRADUATE EDUCATION

The universities involved in our research program, (Caltech, Stanford University, Pennsylvania State University, and University of California at Berkeley) have histories of graduate education, while JPL and the Carnegie Institution are more research- or mission-oriented institutions, with histories of training graduate and postdoctoral fellows on individual projects. This combination offers outstanding opportunities in graduate education.

We will participate in the NASA-sponsored Graduate Student Researchers Program (GSRP). In this program proposals for up to 12 months of research support must be written by the students and submitted with the approval of a potential research sponsor. This is an ongoing, competitive program that will include sponsors from the major NASA centers, and will be available to the members of our Astrobiology Team.

The members of the science team have collectively supervised 27 graduate students in the past 3 years.

C.8.3 POSTDOCTORAL EDUCATION

The postdoctoral fellows supported by this research program will be trained in interdisciplinary science by members of the science team. Their primary training will be “on the job,” working with the co-investigators and doing research. The majority of these postdoctoral fellows will reside at JPL/Caltech, where they will have a JPL/Caltech mentor within our team. One postdoctoral fellow will be resident at Stanford University and will be supervised by Prof. Sleep. The postdoctoral fellows will be supervised jointly by other members of our team at academic institutions (Caltech, Stanford, Pennsylvania State) and research institutions (JPL and Carnegie Institution of Washington) and will have the opportunity to spend some time at different institutions. Given the interrelatedness of the tasks outlined in this proposal the postdoctoral fellows will need to interact frequently with each other, and with many of our team members, resulting in truly multidisciplinary training.

The NAI program offers an unprecedented opportunity for participation to multidisciplinary research. In particular, our postdoctoral fellows will have the opportunity to work with the NAI groups at JPL, Ames, Penn State, and CIW and be exposed to current work in microbiology, field biology, field geology, and theoretical studies in planetary evolution. Providing young scientists with an understanding of the coupling of these disciplines with physical, chemical, and mathematical simulations of planets will be our contribution to astrobiology in the next decade.

In addition, JPL and Ames actively participate in the National Research Council Resident Research Associateship program that supports postdoctoral and senior researchers to come to these institutions. This is a competitive program, advertised by the NRC, that attracts the highest quality researchers. JPL and Ames members of our research program will each write descriptions of their projects for inclusion in the NRC RRA announcement of opportunity.

At CIW, postdoctoral fellows will have access to a diverse spectrum of scientists (geochemists, geophysicists, biologists, material physicists, bio-organic chemists, mineral scientists and planetary scientists), and open access to the wide spectrum of instruments and facilities. Carnegie Institution of Washington funds a Fellows program. There are funds available for 5-6 of these each year. They are one-year appointments, generally renewable for a second year. These are competitively selected on the basis of doctoral thesis research, recommendations, and a research proposal. A seminar visit is generally required also. The selected Fellows are free to carry out the research of their own choosing. They are given open access to the staff and their laboratories and are encouraged to carryout individual cross-disciplinary research.

NAI postdoctoral fellows will be available to us, and we expect having applicants assigned to our research program. We will welcome visiting postdoctoral fellows from other members of NAI to either spend time working with appropriate members of our group, or to interact on research projects via the NGI.

The JPL/Caltech members of the science team have collectively supervised the research of 13 postdoctoral fellows in the past 3 years

C.8.4 Additional Science Team Training Experience

Dr. Vikki Meadows supervises 3 junior scientists at JPL as part of her ongoing NASA Exobiology and Planetary Astronomy tasks.

Dr. David Crisp holds a Bachelor of Science Educational Curriculum and Instruction, in addition to a Ph.D in Geophysical Fluid Dynamics, and is a certified Secondary Education teacher (Texas).

Dr. Ken Nealson directed the NASA Planetary Biology and Microbial Ecology Course for a decade. This course was given at NASA Ames, and featured the teaching of space sciences to biologists, and biology to space scientists. It annually attracted about 20 students and was taught by Nealson and a distinguished group of faculty. The course was originated by Dr. Nealson, and was funded through the exobiology program.

C.8.5 Minority Faculty Program

JPL has an active program called NASA/ASEE, which offers summer faculty fellowships (SFF) for faculty from Historically Black Colleges and Universities (HBCU) and other minority-serving institutions. The SSFs are competitive, and selection is made by the NASA SFF selection committee.

C.8.6 Recruitment

Existing experience within the JPL Astrobiology group indicates that it has been very easy to attract students to multidisciplinary areas like this, and we expect no problems recruiting talented individuals. The opportunity to build an interdisciplinary career working with people of high caliber, and the opportunity to be involved with future space missions are two reasons that recruiting has been and will continue to be rather easy. This, coupled with the network of experts already in place in the Astrobiology community, will help with recruiting.

The recruitment will be different at each level. For undergraduates, we will use established methods, such as the SURF announcements for summer interns, the advertised programs of the PBI program, and college catalogs for course announcements.

At the postdoctoral level, past experience indicates we will attract the highest quality candidates into the program. The existing JPL Astrobiology group has been successful in using advertisements for postdoctoral fellows in astrobiology and has received an overwhelming response in the past from highly regarded institutions. The National Research Council-Resident Research Associateship (NRC-RRA) program will be valuable in both recruitment and selection.

Recruitment of minorities will be achieved via cooperation with JPL's Educational Affairs Office and its Minority Science and Engineering Initiatives. We will also focus some of our efforts on HBCUs and the Hispanic-dominated universities of the Southwest. Finally, we will utilize JPL's Co-op program, which focuses on underrepresented minorities, to engage undergraduates.

C.8.7 Women, Minorities, and Disabled

Recruitment and retention of female, minority, and disabled students will be an important part of our program. Some details have been included in the previous discussion.

Of the two postdoctoral fellows supervised by Prof. Sleep in the past few years, one has been a woman and one was disabled.

The majority of the participants in CIW special programs—summer interns, undergraduate students, postdoctoral fellows, and visiting scientists—are in fact minorities or women at the present time, and CIW actively recruits minority and women candidates.

Finally, as one of the few female principal investigators of an NAI member team, Dr. Meadows will be an important role model for aspiring women astrobiologists.

C.9 Integration of Activities and Role Statements

C.9.1 Principal Investigator

Dr. Victoria Meadows (JPL/Caltech)is the Principal Investigator and is accountable to NASA for the overall research program proposed by this team. Dr. Meadows will ensure that the scientific goals of the program are met and will facilitate interactions and coordination within her team and with other members of the NAI. She will also lead the radiative transfer and climate modeling (Tasks 1-3) and will supervise two post-docs at JPL. She will spend a total of 0.6 WY/yr on these tasks

C.9.2 Co-Investigators

Each co-investigator listed here has participated in the preparation and review of this proposal and has endorsed his or her participation as described here in a letter to JPL (a file of such letters is available on request). In addition to specific investigation responsibilities described below, investigators have allowed time for and will attend the annual meeting and participate in other NAI activities, as appropriate.

Dr. Mark A. Allen (JPL) is the Lead Scientist for Task 4 and 5. He will focus on coordinating the land/ocean/atmosphere interface chemistry and will provide chemical modeling expertise in Task 3. He will spend 0.5 WY/yr of his time on this task.

Dr. Linda R. Brown (JPL) will create a customized database of molecular line parameters which will be used as input for the model calculations. Part of this will be achieved by recording new laboratory spectra for molecules requested by the team members. She will spend 0.23 WK/yr on the task.

Dr. Martin Cohen (UC-Berkeley) will contribute the photospheric spectral energy distributions of main-sequence stars, covering a variety of spectral types, as relevant inputs to the radiative transfer modeling under this proposal. He will also support requisite CAN Team meetings and NAI workshops/ conferences. He will spend 0.12 WY/yr on this effort, for a total of 0.63 WY over the 5-year period.

Dr. David Crisp (JPL) will contribute to the radiative transfer and climate modeling efforts described in Tasks 1 and 2. Specifically, he will take the lead role in the implementation of the radiative transfer models SMART and SMARTMOD. He will participate in the formulation, interpretation, and publication of the experiments using these models in Tasks 1 and 2. He will also collaborate in the efforts to implement these codes on the JPL Ultra-Computing Facilities, and the efforts to integrate these methods into the Virtual Planetary Laboratory (Tasks 3-5). These tasks will require .4WY/yr during each of the 5 years of the proposed effort.

Dr. Amir Fijany (JPL) will collaborate on the analysis of the existing simulation code and its conversion to the appropriate parallel architecture. He will spend a total of .05WY/yr on this task.

Dr. Wesley T. Huntress (CIW) will be the interface for our proposed activity with current activities at the Geophysical Laboratory in early planetary geochemical processes and hydrothermal vent chemistry. The proposal includes 0.05 WY/yr at no cost for Dr. Huntress.

Dr. James F. Kasting (Penn State) will be responsible for supervising the hydrogen escape calculations. These will actually be performed by a postdoc working at JPL. Dr. Kasting will also supply information from his ongoing photochemical modeling work that is being carried out under separate funding from NASA Astrobiology and Exobiology. These two efforts combined will occupy about 30 percent of Dr. Kasting's time. He anticipates spending a minimum of 5% of his time to this research program. However, there is no direct charge to this proposal, other than the support requested for the JPL postdoc.

Dr. Cherilynn A. Morrow (Space Science Institute) will work with the PI to manage the education and public outreach (EPO) aspect of the proposal. The plan involves educator workshops, public symposia, and web-based resources. Implementation will engage proposal scientists in partnership with several other EPO organizations whose involvement will be coordinated by Morrow. She will spend approximately .1WY/year on this task.

Dr. Ken Nealson (JPL) will be responsible for providing constraints on the production of biogenic gases by various forms of life. He will also act as liaison with Dr. Dave DesMarais' group at NASA Ames. He will spend a total of .05WY/yr of his time on these tasks.

Dr. Mark Richardson (Caltech) will lead the development of atmospheric loss models for the Global Model and the Virtual Planetary Laboratory. He will also provide general support for coupled global model development and testing, and support requisite CAN Team meetings and NAI workshops/ conferences. He will spend 0.25 WY/yr on this effort, for a total of 1.25 WY over the 5-year period.

Dr. Rob Rye (Caltech) will be responsible for the development of parameterization schemes for global fluxes of various biogenic gases as a function of environmental variables. He will spend 0.5 WY/year on this task.

Dr. Norm Sleep (Stanford) Prof. Norman Sleep will supervise the development of mechanistic descriptions of global geochemical cycles and their effects on planetary atmospheres for inclusion into the Virtual Planetary Laboratories. He will devote .1WY/yr of his time to this activity.

Dr. Michael Storrie-Lombardi (JPL) will implement the multi-sensor Bayesian classification and analysis algorithms for the biosignatures spectral catalog. He will also coordinate analysis of the modeling software for migration to a parallel ultracomputing architecture. He will spend .20 WY/yr on this task.

Dr. Thangasamy Velusamy (JPL) will investigate the detectability of the biogenic spectral features by modeling the performance of future space missions such as Terrestrial Planet Finder (TPF). He will spend 0.1 WY/yr on this task.

Prof. Yuk L. Yung (Caltech) will participate in the development and application of the photochemical and evolution models for studying the interactions between the atmosphere and the biosphere. While most of the chemical modeling tools have been built by his group in the last twenty years, he will have to modify them for application to Astrobiology, with particular emphasis on the coupling between the atmosphere, ocean, biosphere and escape processes. He will spend 0.1 WY/yr of his time on this task.

Dr. Kevin Zahnle (NASA-Ames) will supply descriptions of impact processing of planetary atmospheres for incorporation into atmospheric chemistry models. He will also work with others in parameterizing geophysical cycles that in part control the atmospheric abundances of important volatile compounds. He will spend 0.1 WY/yr on this task.

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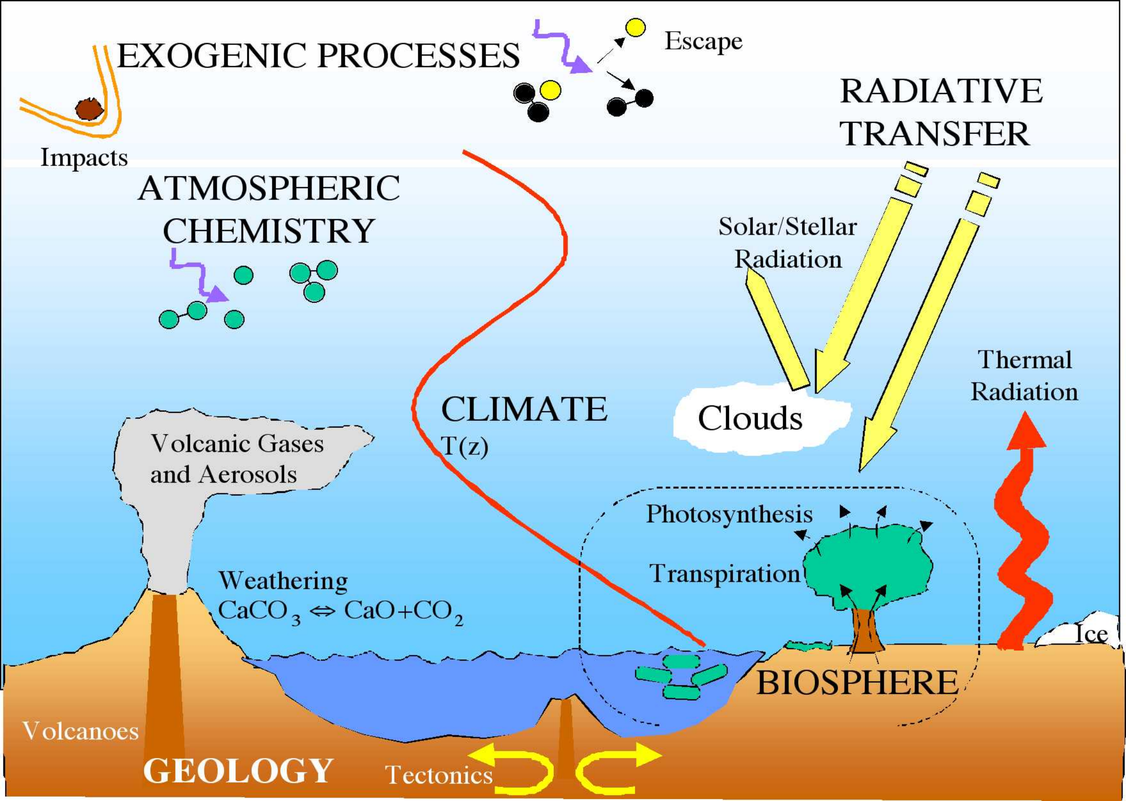
EXOGENIC PROCESSES
Escape
Impacts
RADIATIVE
TRANSFER
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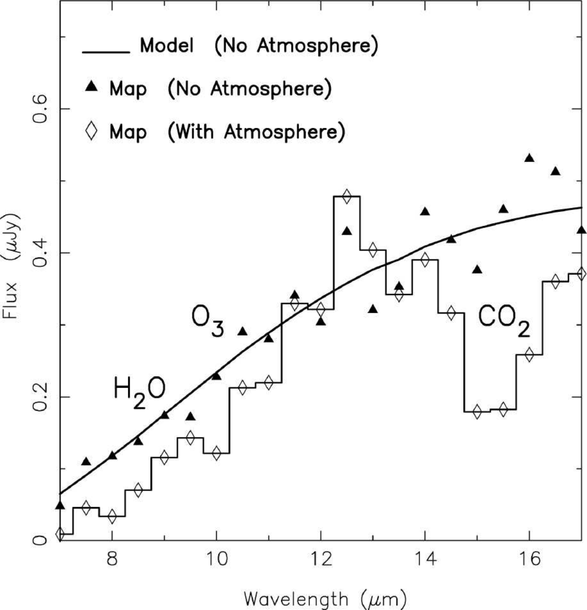
Model (No Atmosphere)
Map (No Atmosphere)
Map (With Atmosphere)
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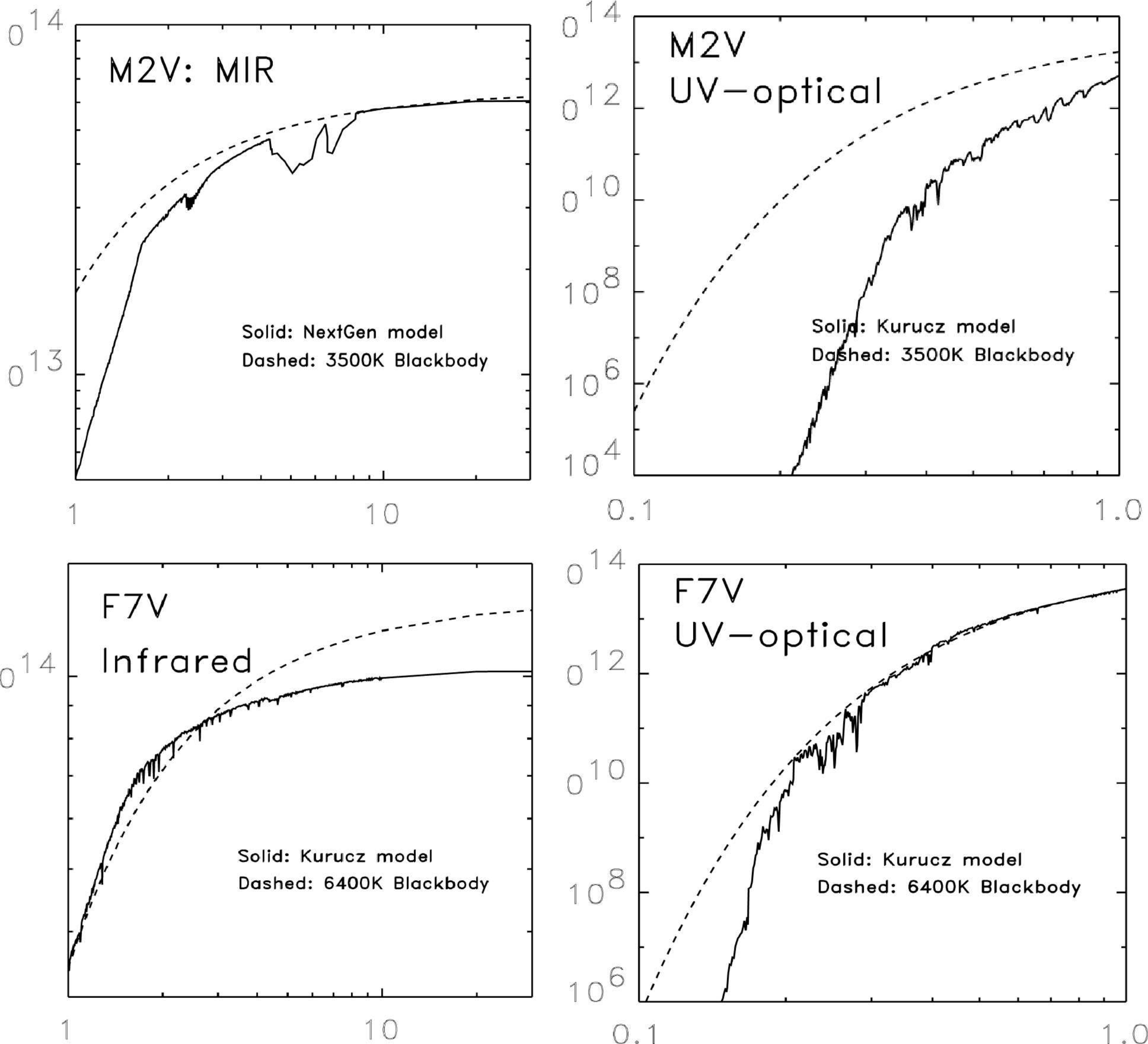
Wavelength (μm)



M2V: MIR
Solid: NextGen model
Dashed: 3500K Blackbody
M2V
UV–optical
Solid: Kurucz model
Dashed: 3500K Blackbody
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Infrared
Solid: Kurucz model
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F7V
UV–optical
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