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**VALIDATION OF A RADIATIVE TRANSFER MODEL FOR THE
ATMOSPHERE OF THE GIANT PLANETS THROUGH THE DATA
OF VIMS (VISIBLE INFRARED MAPPING SPECTROMETER)
THE IMAGE SPECTROMETER OF THE CASSINI-HUYGENS
INTERPLANETARY MISSION**

VALIDAZIONE DI UN MODELLO DI TRASFERIMENTO RADIATIVO PER L'ATMOSFERA
DEI PIANETI GIGANTI MEDIANTE I DATI DELLO SPETTROMETRO AD IMMAGINE
VIMS (VISIBLE INFRARED MAPPING SPECTROMETER) DELLA MISSIONE
INTERPLANETARIA CASSINI-HUYGENS

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Abstract

The aim of this work is the construction and validation of a Radiative Transfer model for the Giant Planets atmosphere using the data of the image spectrometer VIMS, instrument on board the spacecraft of the Cassini-Huygens mission to Saturn.

The Cassini mission to Saturn is one of the most ambitious mission in planetary space exploration ever and the spacecraft is one of the largest, heaviest and most complex interplanetary spacecraft ever built.

Mainly it is composed by a two part structure: the Cassini orbiter and the Huygens probe. This last element is deputed to get into the Titan's atmosphere, landing on the planet. The first element of the entire spacecraft is designed to enter in orbit around Saturn, deliver the Huygens probe to its final destination and conduct at least four years of detailed studies of Saturn's system.

VIMS is a remote sensing instrument designed, built and developed for the Cassini mission to Saturn by an international team representing the national space agencies of different countries.

The instrument's unique system design consists of two different spectrometers actually: VIMS-V for the visible part of the electromagnetic spectrum and VIMS-IR for the near infrared part, covering a total wavelength range from $0.35\ \mu\text{m}$ to $5.1\ \mu\text{m}$ with 352 channels.

VIMS-V and VIMS-IR are different for many technical aspects but they work in unison to provide data set that appears as if it were made by a single device.

VIMS data are called cube, normally used for storing data produced by imaging spectrometers.

The name cube is absolutely without any real physical meaning. It is only an informatic architecture, a conceptual or "logical" view of the data itself.

The main informations are stored in the "core" of the structure. The core region of the cube data object contains the main data array that is being stored inside. Being VIMS an image spectrometer, the core consists of a number of spatial image planes corresponding to a different wavelength bands.

Once the measured data are available however, we need to produce a model which properly simulate what the instrument measures in order to retrieve specific parameters and to get information on the atmosphere in general.

The code we use for our purpose is ARS (Atmosphere Radiation Spectrum).

Basically, it is a set of routines written in fortran 77 and C able to perform computations of several physical quantities and to solve the radiative transfer equation under

different conditions.

Using different packages separately, the code can compute the opacity of gaseous species and aerosols, the transmittance and the radiance spectra.

As starting point for the generation of synthetic spectra, the first task is to specify a self-consistent pressure–temperature profile for the atmosphere of Saturn.

We adopted one of the profiles used for the analysis of the Cassini - CIRS data. This profile is able to reach only the 4 *bar* level. The temperatures at pressures larger than about 4 *bar* have been obtained by extrapolation of this temperature profile according to a dry adiabatic.

In order to simulate the atmosphere of Saturn, our model takes into account the main molecules which the atmospheres of Giant Planets are made of.

The atmosphere is modeled as a mixture of eight different gases: CH₄ (considering separately its three isotopes ¹²CH₄, ¹³CH₄, CH₃D), H₂O, NH₃, PH₃.

H₂ and He has been also considered to define the *continuum* level of IR emission. All these species are spectroscopically and optically active in the bandwidth of the instrument.

The mixing ratios of the considered species are constant in altitude, with the exception of NH₃, PH₃ and H₂O.

The first step using a line-by-line code is the choice of the grid for the simulation. This is a very important step, being computation time dependent on chosen resolution. In order to reproduce the signal of the instrument, the wavenumber grid covers all the bandwidth, between 1880 *cm*⁻¹ (5.32 *μm*) and 10⁴ *cm*⁻¹ (1.0 *μm*).

After the definition of the molecules, their abundances, the thermal profile, the resolution of the grid and other parameters, we have run the code to generate the absorption coefficient of all the species involved.

Given the absorption coefficients of the various gases in the atmosphere, the emerging radiance for a real atmosphere can be calculated through the calculations of transmittance.

Having the instruments onboard spacecrafts and satellites spectral resolutions lower than those available on ground base instruments, synthetic spectra calculations are compared with real measured spectra which very often do not need high resolution spectra to be compared with.

In order to compare the simulated radiance spectra with the real ones, a convolution of line-by-line ARS outputs on the instrumental grid was needed.

The radiance, computed by ARS at high spectral resolution, has been convolved with a Gaussian function, gridded on the instrument's channel wavenumber and then adapted to the wavelength units, in order to have the resulting spectrum in equally spaced wavelengths as the comparison with VIMS requires.

All the calculations have been done using the Full Width Half Maximum (FWHM) taken from the official ancillary data header file, linked to the observations. Actual atmospheres are not only a mixture of molecules in gaseous phase.

Particles of different size, shape, composition and lifetime substantially modify the spectral behavior observed by any instrument.

In order to obtain physical informations under more realistic condition from spectral analysis, is very important to simulate the presence of aerosols and particles in the atmosphere.

According to the most recent theoretical thermochemical modeling [81], the Saturn's upper atmosphere is expected to contain three main cloud layers:

- An ammonia (NH_3) ice crystal layer centered at near $1 \div 1.5 \text{ bar}$
- An ammonium hydrosulfide layer (NH_4SH) centered at near $3 \div 4 \text{ bar}$
- A water layer centered at $8 \div 10 \text{ bar}$

The actual locations are uncertain because of the unknown abundances of the condensing constituents.

Above the ammonia cloud however, thin hazes extend up to few *mbar*.

In the stratosphere the aerosols formation is driven by photolysis processes.

Methane (CH_4) is a significant minor constituent of the stratosphere of Saturn. Photolysis of methane by solar radiation yields various product hydrocarbons of which the most abundant are ethane (C_2H_6) and acetylene (C_2H_2). Neither of these molecules however should exist under thermochemical equilibrium.

Models of methane photochemistry show a coupling between ethane and acetylene leading to more complex polycyclic aromatic hydrocarbons (PAHs).

The increase of temperature with height in the stratosphere implies the presence of additional energy sources. These sources include absorption of ultraviolet radiation from the Sun via gaseous photodissociation reactions and by stratospheric aerosols.

Thus the temperature structure in the stratosphere depends critically on the vertical distribution of photochemical products in the same way that the stratospheric temperature profile of the Earth depends critically on the abundance of another photochemical product; the *Ozone* (O_3).

At deeper levels, the water cloud is more massive and is more likely to be convective and sporadic with small areal coverage.

Studies based on cumulus parameterization show that water-based moist convection would occur on the giant planets and create a stable layer over a depth of about a scale height above the water condensation level. This putative stable layer is too deep to have been observed but is crucial to many shallow weather layer theories of Giant Planet circulations.

The interpretation of observational data seems to indicate that a simple atmospheric model consisting of a reflecting cloud layer beneath an absorbing gas layer or a vertically homogeneous distribution of scatterers, cannot describe satisfactorily the observations.

The enrichment and/or depletion of the higher cloud as well as the deeper can be seen from the analysis of the spectra and from the images.

The expected vertical distributions and compositions of tropospheric clouds from thermochemical equilibrium theory and stratospheric haze from photochemistry, shows how different cloud layers are responsible for the observed spectrum of Saturn.

Because the solar part of the VIMS spectra is very sensitive to the aerosols vertical distribution in the upper troposphere and lower stratosphere, the effect of how different levels of aerosols and clouds affect the signal has been considered in the range between $1 \mu\text{m}$ and $3.2 \mu\text{m}$.

In the thermal range between $4.4 \mu\text{m}$ and $5.2 \mu\text{m}$, where the instruments sounds the deep atmospheric levels, the model reveals the need for thick deep clouds in order to

fit the data.

In order to retrieve physical parameters from the comparison with the actual data of the observations, we have create a high resolution synthetic spectra databank in the range between $1\ \mu m$ and $5.2\ \mu m$, covering the whole instrument bandwidth.

For a given set of initial model free parameters we have calculated the synthetic radiance data for different observation geometry, comparing the results with the chosen observations at the same geometry.

A least squares fit has been used to reach the best fit between the actual data and the elements of the databank.

One of the main aspect of the VIMS data is the great variability of the measured spectra both in visible and infrared channel.

If we consider the behavior of typical VIMS-IR spectra as recorded by data, the images reveal three major latitude regimes: the polar regions, the middle latitudes and the equatorial zone.

Three images at these three different latitude are considered in order to test the model.

The spectra are strongly influenced by clouds and aerosols and reveal two major vertical regimes: the stratospheric zone above the interface with the troposphere near $100\ mbar$ and the troposphere itself.

The auroral processes drive the chemistry of the planet in the polar regions north of about 60° , here a stratospheric haze is optically thicker and darker than stratospheric haze at other latitudes.

At mid-latitude deep tropospheric clouds which probably form in free convection display substantial seasonal and nonseasonal variations. Distinct hazes layers at some latitudes are revealed by high spatial resolution limb images as well.

After the comparison between our data and the VIMS ones, it is evident how the model cannot give an unique solution but only the best combination of all the *a priori* parameters able to fit better the instrument spectra.

The equatorial zone is a region of consistently high clouds and thick haze. In this case our model is not able to reproduce the measured signal over the entire instrument range, anyway we found that the size of the particles is bigger than at other latitudes. Both stratospheric and tropospheric particles are located higher in altitude and this region seems not to be populated with clouds but an uniform sheet seems to cover the region, possibly because of strong zonal wind shear.

At middle latitudes before -60° the first principal variation in occurs.

Here, our model predicts smaller particles with the base of the clouds located at lower pressures with respect to the equatorial region. The opacity become lower for both the stratospheric and tropospheric clouds.

At this latitudes, atmospheric areas with a complete different deep clouds structures show the same spectral behavior in the solar part of the instrument range between near $1\ \mu m$ and $3.2\ \mu m$. The different deep clouds structures are well visible in the thermal range between $4.4\ \mu m$ and $5.2\ \mu m$ and in the images at $5.1\ \mu m$ as well.

The base clouds pressures after this boundary at near -60° increase with latitude moving to the South Pole, with the pressures in general being bigger than those before the boundary for both the stratospheric and tropospheric clouds.

After the boundary the size of the particles become smaller and the optical thickness

decreases in the analyzed region.

Besides pressure variations in the upper cloud layers, we also find for that particular regions before the boundary, the most high opacity for the deeper clouds than the other observations.

At polar latitudes, for the analyzed image the pressure of the stratospheric haze appears to increase, the model shows an equal set of parameters for all the simulated spectra of every observation. It seems again that an uniform cap made of a thin stratospheric haze covers the southern polar regions.

The tropospheric clouds extend probably lower than the same clouds at other latitudes and the same values for the size of particles at mid-latitudes after the boundary at -60° are found.

As said before, the retrieved vertical structure of the atmosphere and its latitudinal variation must to be considered only as the best set of parameters that fit the actual data.

We can say nothing about the actual size and/or pressure levels of the upper stratospheric haze or the tropospheric and deeper clouds. Moreover, just to test the model we consider only one observation for every planetary bands, and the outputs can't be really considered as a general behavior.

In order to make the model complex a number of different changes are planned for the future as well.

Anyway, the results of this work seem to support the idea that our model is able to reproduce the signal of the instrument and give indications about some physical constraints of the vertical aerosols and clouds profile inside the range of the *a priori* fixed parameters.

We remark that even if the model has been made with the aid of some simplifying assumptions and validity conditions, our results are in agreement with the results obtained by other studies, and this agreement is remarkable considering the very different techniques used in the different works and the most complexity of the other models.

Compendio

L'origine del sistema solare è uno dei problemi fondamentali della scienza.

Unitamente ad altri quesiti come l'origine dell'Universo e la formazione delle galassie, rappresenta un punto cruciale per la comprensione della nostra stessa esistenza.

Le prime ipotesi sulla formazione del sistema solare vanno fatte risalire agli studi di Kant e Laplace, che definirono la teoria nebulare, secondo la quale, circa 4.5 miliardi di anni fa una nube di gas interstellare, iniziò a collassare.

La parte centrale, in seguito alla contrazione gravitazionale propria, iniziò a riscaldarsi fino a quando, reazioni termonucleari interne, iniziarono a rilasciare l'energia prodotta nello spazio circostante. Con la diminuzione della temperatura, una parte del materiale più interno, iniziò a condensare in singole particelle di materia che, a causa di effetti gravitazionali e complesse sequenze di mutui disturbi e interazioni, portarono alla formazione dei pianeti e dei corpi che possiamo osservare oggi.

Negli anni '50 e '60 tuttavia, una rivisitazione profonda della teoria iniziale è stata operata, principalmente da Safronov e Schmidt, a causa delle nuove e profonde osservazioni sia teoriche che sperimentali, che hanno portato a delle correzioni sullo scenario in precedenza ipotizzato.

Le recenti scoperte di dozzine di pianeti giganti extrasolari posti ai confini estremi del nostro sistema e con proprietà in generale differenti, hanno sollevato questioni e dubbi circa la validità del modello formativo.

L'importanza di studiare i pianeti giganti quindi risiede nel fatto che questi corpi, oltre a fornire importanti indizi proprio sulla formazione del nostro sistema solare, la loro composizione chimica, infatti, è fortemente legata alla quantità d'elementi presenti nel gas contenuto nella nube solare primordiale, rappresentano un elemento di paragone per quelli extrasolari, portatori di informazioni evolutive differenti.

Atmosfere dei pianeti giganti

Costituiti in sostanza da gas, i pianeti più esterni del nostro sistema solare sono privi di una vera e propria superficie di separazione, come avviene per i pianeti terrestri, e l'assenza di questa interfaccia, genera la necessità di definire cosa si intenda per atmosfera.

Si può tuttavia ragionevolmente indicare come atmosfera in senso proprio, la regione che si estende, verticalmente, dal livello d'alcuni *mbar* fino ad alcune decine di *bar* di pressione, questo anche in considerazione del fatto che quella indicata, risulta essere

la regione maggiormente accessibile per le osservazioni e quindi la meglio conosciuta. Investigazioni spettroscopiche nell'ultravioletto, dove la maggior causa di opacità è dovuta allo scattering Rayleigh, forniscono informazioni sui livelli più esterni (alcuni μbar), mentre la luce solare riflessa dalla sommità delle strutture esterne, che domina le indagini nel visibile e nel vicino infrarosso, sonda gli strati intermedi (alcuni bar), infine l'indagine infrarossa vera e propria e quella delle onde radio, per interpretare le strutture dei livelli più profondi, posti a decine di bar di pressione.

Anche se la composizione dell'atmosfera dei pianeti giganti, è completamente dominata da H_2 ed He , diversi altri elementi e composti sono stati identificati nel corso delle osservazioni: CH_4 , NH_3 e PH_3 , altri composti come l'acqua (H_2O), l'acido solfidrico (H_2S), oppure elementi come il deuterio (D) nella forma di metano deuterato CH_3D o il Germanio (nella forma GeH_4).

Altri composti si formano dagli elementi citati, come l'idrosolfato d'ammonio (NH_4SH) o l'idrossido d'ammonio (NH_4OH). Carbonio (C) ed azoto (N), nelle forme di monossido (CO) o biossido (CO_2) per il primo e nella forma molecolare (N_2) per il secondo. Sono stati individuati positivamente inoltre, anche gli idrocarburi, tra cui citiamo l'acetilene C_2H_2 o l'etano C_2H_6 .

Dalle misure delle abbondanze delle specie minori rilevate, è possibile calcolarne i rapporti relativi alla specie maggioritaria, tipicamente idrogeno (H_2).

Tali calcoli, risultano relativamente semplici quando le specie sono ben mescolate, il loro rapporto allora risulta costante attraverso tutta la regione atmosferica considerata.

E' il caso di specie non facilmente condensabili, come CH_4 ed il CH_3D i cui rapporti, in funzione dell'idrogeno, rimangono costanti con l'altitudine, *vice versa* in altri casi, tale rapporto varia con la quota a causa dei processi fisici e chimici che intervengono, come la condensazione, come avviene per H_2O e NH_3 o la fotodissociazione per specie come NH_3 e PH_3 o reazioni chimiche, che interessano PH_3 e GeH_4 .

La conoscenza delle specie presenti, è di fondamentale importanza in ordine di stabilire, a partire dai modelli termodinamici, la composizione e i livelli di nubi, in funzione della pressione (altitudine). Tali livelli, sono una parte importante del bilancio energetico globale, costituiscono infatti una superficie parzialmente riflettente per la luce solare, una causa di opacità nell'assorbimento della radiazione esterna ed una barriera per la fuoriuscita del flusso planetario, costituendo inoltre una sorgente di radiazione infrarossa termica.

Il bilancio termico cioè viene influenzato dalla formazione delle nubi, considerando anche il riscaldamento prodotto dal calore latente di condensazione e dal ruolo primario che tali strutture giocano nella formazione di tempeste e nella meteorologia in generale. Dall'individuazione della presenza di un composto allo stato gassoso inoltre, usando la curva di saturazione della specie, la sua abbondanza e conoscendo il profilo termico planetario, risulta possibile ricavare il livello atmosferico al quale la specie condensa in strutture nuvolose.

Sfortunatamente l'esatta composizione delle strutture non è di facile soluzione attraverso le tecniche remote, mentre misurazioni *in situ* di profondità, mediante sonde penetranti, forniscono profili reali pur essendo più difficili da realizzare.

La missione Cassini-Huygens

Quella della Cassini-Huygens rappresenta un ritorno al sistema Saturno dopo le missioni Pioneer e Voyager degli anni settanta.

L'idea della missione affonda le proprie radici nei primi anni '80 quando venne ipotizzata la possibilità di una collaborazione tra America ed Europa circa l'esplorazione spaziale planetaria.

La missione prevedeva l'utilizzo congiunto di un orbiter e di un lander (per la discesa sulla superficie di Titano).

Gli obiettivi scientifici pianificati, evidenziavano l'esigenza di investigare il sistema Saturno nel suo insieme ma anche di esplorare precisi siti del sistema, utili alla comprensione di molti fenomeni fisici riscontrabili in altri sistemi planetari.

La missione avrebbe avvicinato il sistema Saturno, e Titano in particolare, circa trecentocinquanta anni dopo le prime osservazioni dalla terra da parte di due illustri astronomi del XVII° secolo: Gian Domenico Cassini scopritore, fra il 1671 ed il 1684, di quattro satelliti di Saturno e successivamente di una lacuna negli anelli e Christiaan Huygens scopritore, nel 1655, proprio di Titano, il più grande tra i satelliti di Saturno.

Partita il 15 ottobre del 1997, la sonda raggiunge, nel luglio del 2004, il suo obiettivo finale dopo un viaggio di circa 7 anni. La necessità di sfruttare manovre di gravità assistita, per il raggiungimento della meta finale, ha portato la sonda ad effettuare diversi 'fly by' durante il viaggio. Proprio nell'ultima di queste manovre, nel dicembre 2000, avviene l'incontro con Giove.

Con un tempo nominale di quattro anni, la missione di Cassini venne quantificata in circa 70 orbite dal disegno fortemente ellittico al fine di ottimizzare proprio la quantità di obiettivi fisicamente osservabili dagli strumenti ospitati sulla sonda.

Tra gli obiettivi bisogna certamente considerare *in primis* l'atmosfera di Saturno, che costituisce uno degli obiettivi primari, a causa sia della complessità della dinamica che per la natura della sua composizione chimica.

La distribuzione delle specie presenti, il comportamento in scala temporale dei venti e dei vortici superficiali, la distribuzione delle temperature zonali, lo studio delle strutture e dei fenomeni di convezione dagli strati più interni nonché la natura dell'emissione termica di Saturno solo alcuni dei campi d'interesse correlati.

Bisogna considerare che la necessità della missione trova sostegno nella incompletezza delle informazioni ottenute dalle missioni precedenti. Osservazioni caratterizzate da passaggi delle sonde sul target senza una sequenza orbitale sufficiente a pianificare molteplici acquisizioni unitamente a tempi relativamente piccoli di osservazione non permisero, infatti, il rilevamento di alcuni fenomeni atmosferici, proprio a causa dei lunghi tempi dinamici delle strutture superficiali.

La possibilità di disporre di orbite differenti, permette al contrario di studiare variazioni latitudinali, longitudinali e temporali di molte strutture atmosferiche.

Tra le principali finalità delle osservazioni trovano posto la determinazione della distribuzione verticale, al variare di latitudine e longitudine, delle diverse specie gassose presenti o la variazione temporale dei composti chimici non in equilibrio.

Potenziali indagini eseguite sia nel visibile che nell'infrarosso possono evidenziare le strutture nuvolose, il sistema di circolazione atmosferica del pianeta e la fisica zonale.

La maggior durata delle osservazioni permette, inoltre, uno studio della distribuzione

alle varie altitudini delle specie attive, di tracciare un profilo di temperature, di studiare le abbondanze relative dei costituenti minoritari, le proprietà microfisiche degli aerosols e le loro proprietà diffusive.

Inoltre, studi paralleli sulla meteorologia saturniana, sulle tempeste che si generano, studi sulla natura degli 'hot spots' e 'cold spots' e sulla composizione delle macchie e degli ovali. Oltre al pianeta, gli obiettivi scientifici sono incentrati anche sul sistema dei suoi anelli.

Una magnificenza unica in tutto il sistema solare, estremamente importante per la comprensione dei fenomeni di aggregazione del materiale orbitante. L'ingresso della sonda fra gli anelli, ha offerto la possibilità di investigare le proprietà di diffusione delle particelle stesse.

È importante focalizzare la specifica morfologia e composizione, la distribuzione dei costituenti e le loro dimensioni, la variazione delle strutture e le polveri. Precedenti osservazioni hanno, infatti, messo in luce notevoli differenze tra i vari anelli. Altre informazioni inoltre riguardano le onde di densità all'interno del sistema di anelli ed altri effetti dinamici in generale.

Anche i satelliti risultano oggetto di indagine, rappresentando l'occasione di studiare le complesse fenomenologie geologiche che hanno (e hanno avuto) luogo, come fenomeni di vulcanismo ghiacciato.

Possibili analisi degli accrescimenti occorsi in seguito alla devastazione della superficie primordiale a causa dell'intenso bombardamento meteorico.

Non tutti i satelliti di Saturno sono stati generati con il sistema stesso ma alcuni verosimilmente sono oggetti catturati dal campo gravitazionale del pianeta. Si offre la possibilità quindi di analizzarne la composizione, la dinamica e gli effetti gravitazionali connessi con il sistema che li avrebbe catturati e l'origine.

Fra i satelliti una menzione a parte la merita Titano.

Se un obiettivo primario era lo studio del sistema pianeta-anelli, non era da meno l'investigazione di questo satellite.

L'interesse era così evidente che il lander ne è la prova.

Una missione nella missione.

L'ingresso nell'atmosfera di Titano, la più simile a quella terrestre, della sonda Huygens ha fornito indicazioni dirette sulla composizione delle specie e sulla distribuzione degli aerosols. Per l'atmosfera in generale, valgono le stesse opportunità di indagine elencate per Saturno.

Infine, la geologia e la morfologia della superficie, in particolar modo quella del punto di impatto con la possibilità di un'analisi *in situ* unica, unitamente a tracce di attività tettonica e vulcanismo.

VIMS (Visibile Infrared Mapping Spectrometer)

Come indica il nome stesso, questo strumento è uno spettrometro in grado di acquisire, simultaneamente, immagini e spettri di una stessa regione spaziale mediante due canali operanti in prefissati intervalli spettrali.

Sostanzialmente è composto da due spettrometri indipendenti: VIMS-V, canale visibile e VIMS-IR, canale infrarosso, in grado di lavorare in modo complementare per fornire informazioni visive e spettrali in entrambi gli intervalli di lavoro.

Pensato e realizzato per l'analisi della radiazione emessa e riflessa, VIMS è in grado di catturare immagini, in 352 colori (lunghezze d'onda prefissate) nello stesso istante, con un range che, complessivamente, si estende da $0.35 \mu m$ a $5.1 \mu m$.

I due canali operano in modo totalmente diverso, pur fornendo due dati equivalenti da un punto di vista 'dimensionale'.

In generale, il dato prodotto è un'immagine acquisita, per entrambi gli spettrometri, con un FOV nominale di 64×64 pixel, ciascuno dei quali ottenuto mediante la composizione degli IFOV, differenti per i due strumenti. Il singolo pixel che costituisce l'immagine, che ciascun rivelatore ricostruisce, è un quadrato di $500 \times 500 \mu rad$. A causa del diverso dimensionamento degli elementi preposti all'acquisizione però, la ricostruzione dell'immagine avviene in due modi distinti.

VIMS-V acquisisce l'immagine nominale in modalità 'push-broom', osservando un'intera riga di 64 pixel per volta, per poi passare alla riga successiva. Per costruire tutta l'immagine, la CCD viene letta dopo ogni riga acquisita mentre lo specchio di scansione passa, uniformemente, alla successiva. L'IFOV pixel di VIMS-V 'è un quadrato di $167 \times 167 \mu rad$.

Diversamente, VIMS-IR possiede un rilevatore lineare ed è in grado di generare dati acquisendoli in modalità 'whiskbroom'. Osserva quindi, non tutta una linea per volta ma un singolo IFOV pixel ($250 \times 500 \mu rad$) per esposizione che viene, successivamente, sommato ai precedenti per ricostruire tutta la scena del target lungo quella riga.

La risoluzione media spettrale risulta essere, rispettivamente per VIMS-V e VIMS-IR, di $7.3 nm$ e $16.6 nm$. In accordo con lo standard PDS (Planetary Data System), i dati ottenuti da VIMS sono delle strutture a tre dimensioni, chiamate 'cubi' in cui ad ogni 'lato' corrisponde un ben preciso parametro misurato.

Delle tre dimensioni, due sono tipicamente costituite da coordinate spaziali e la terza corrisponde a quella spettrale (valori di lunghezza d'onda).

Lo strumento è deputato a misurare riflettanze di oggetti investiti dalla luce solare o la radiazione termica emessa nel vicino infrarosso. Una volta calibrati, i cubi ottenuti forniscono quindi 352 immagini, una per canale, di 64×64 pixel. Per ogni pixel possiamo ricavare lo spettro dei valori di riflettanza banda per banda.

Finalità della ricerca

Scopo principale della ricerca è quello di sviluppare un modello di Trasferimento Radiativo per le atmosfere dei pianeti giganti e convalidarlo mediante i dati dello strumento precedentemente descritto.

A dispetto del titolo della tesi tuttavia, il modello è stato testato solo sui dati VIMS relativi alle acquisizioni di Saturno.

Nel caso di Giove, i dati acquisiti durante il *fly-by* nel Dicembre del 2000, sono risultati non sufficientemente risolti spazialmente per gli obiettivi prefissati.

La convalida del modello infatti prevede la necessità di avere immagini sufficientemente risolte spazialmente, per poter discriminare aree relativamente vicine ma con comportamenti spettrali differenti. A causa della grande distanza dello spacecraft dal pianeta durante le acquisizioni su Giove però, i valori di radianza misurati risultavano mediati su aree troppo estese per poter fare delle simulazioni mirate.

Il modello di Saturno, definito mediante una caratterizzazione chimico-fisica, dinam-

ica e spettroscopica con delle condizioni imposte a priori, ha consentito la realizzazione di spettri sintetici simulanti la risposte di uno strumento come VIMS. La bontà delle scelte fatte si ripercuote sul confronto tra i dati sintetici e quelli realmente misurati dallo strumento.

Pur essendo la validità del modello in generale l'obiettivo principale della ricerca, altre finalità sono state considerate:

- Analisi di immagini a diverse latitudini per caratterizzare scenari differenti dell'atmosfera in oggetto.
- Creazione di un database spettrale di riferimento contenente spettri simulati con diverse parametrizzazioni.
- Effetti delle nubi sul segnale simulato e loro caratterizzazione fisica come quota di persistenza (pressione) e proprietà ottiche (raggio particelle, opacità) in funzione delle osservazioni.

Tutta la metodologia riguardante il modello viene sorretta dall'implementazione di un codice scritto per automatizzare il riconoscimento dei parametri fisici della simulazione da riferire al segnale misurato. Tale codice viene scritto con procedure IDL e fa riferimento a script bash per l'esecuzione in ambiente linux.

Il modello

Punto di partenza è stata la creazione di spettri sintetici delle quantità necessarie alla soluzione dell'equazione del trasferimento radiativo in atmosfera.

Il codice utilizzato è ARS, sviluppato da N.I. Ignatiev (IKI/RAN - IFSI/INAF). Fondamentalmente è costituito da un pacchetto di programmi che implementano un calcolo esatto *line-by-line* del coefficiente d'assorbimento delle principali molecole.

Da questi coefficienti è possibile allora ricavare altre quantità usate nel calcolo del trasferimento radiativo come l'opacità dei gas e degli aerosol, la trasmittanza, la radianza ed altre quantità a queste correlate.

Il programma è scritto in linguaggio Fortran 77, con l'ausilio di funzioni del Fortran 90 e C.

Dopo l'acquisizione delle informazioni disponibili da database di pubblico dominio circa gli elementi e le molecole coinvolte, la posizione e l'intensità delle linee spettrali, il valore dei coefficienti d'allargamento delle stesse, le energie nello stato fondamentale, le probabilità di transizione, nonché la definizione di altri parametri rilevanti, la ricerca è continuata allo scopo di caratterizzare al meglio, da un punto di vista spettroscopico, le atmosfere in oggetto.

Lo studio spettroscopico è stato eseguito in maniera generale, completando via via le parti non ottimali o, peggio, mancanti. Sono state tuttavia considerate le seguenti molecole: CH₄ (considerando separatamente i suoi isotopi ¹²CH₄, ¹³CH₄, CH₃D), H₂O, NH₃, PH₃. H₂ e He sono stati considerati per definire il livello del continuo.

Il range spettrale considerato è quello della banda passante di VIMS-IR (1.0 μm 5.2 μm).

Dai dati dello strumento CIRS, ospitato a bordo dello spacecraft Cassini, è stata

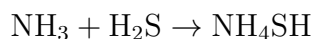
implementata la struttura termica (profilo pressione temperatura) dell'atmosfera saturniana.

L'approssimazione di atmosfera piana e parallela è stata adottata.

Per la costruzione dei profili di nubi è stato usato un modello di condensazione verticale che partendo da una composizione solare calcola le abbondanze di aerosols in atmosfera.

Tre diversi livelli di nubi sono stati considerati:

- **Foschia stratosferica** [1 *mbar* - 60 *mbar*]: E' composta dai prodotti della fotodissociazione del metano in alta atmosfera ad opera dei raggi ultravioletti e mediamente è situata tra pochi *mbar* e alcune decine. E' responsabile della maggior parte della riflessione solare e del segnale misurato dallo strumento tra 1 μm e circa 3 μm .
- **Nubi troposferiche** [100 *mbar* - 1 *bar*]: Alla temperatura di circa 140 *K*, l'ammoniaca NH_3 condensa in nubi di ghiaccio. La parte più alta, e visibile, delle nubi di Saturno è rappresentata da strutture ghiacciate costituite da ammoniaca.
- **Nubi profonde** [2 *bar* - 5 *bar*]: per temperature prossime ai 230 *K*, NH_3 e H_2S si ricombinano e condensano tramite la reazione:



formando l'idrosolfato d'ammonio. La conseguente formazione di nubi, possiederà una locazione verticale che dipende principalmente dall'abbondanza relativa degli elementi in questione. A causa della reazione mostrata, la specie con abbondanza minore tra le due, per Saturno H_2S , risulta praticamente rimossa dall'atmosfera. Questo spiegherebbe perché l'acido solfidrico non è stato rilevato con le tecniche remote. La sonda di profondità *Galileo*, per Giove, ha verificato positivamente, la presenza di tale gas ma a pressioni maggiori. L'ingresso nell'atmosfera di Saturno, di una sonda analoga, proverebbe la veridicità delle assunzioni.

La foschia stratosferica è stata modellata come una mistura di N_2 - CH_4 , le nubi troposferiche con ghiaccio di ammoniaca e le nubi profonde con ghiaccio di idrosolfato d'ammonio.

Per le particelle profonde un raggio efficace di 40 μm è stato adottato per garantire la risposta più piatta possibile nel range termico. Le particelle di ghiaccio che formano le nubi sono state considerate delle sfere e le proprietà ottiche sono state calcolate in approssimazione di Mie.

Sulla base di queste informazioni sono state ricavate l'opacità dei gas e degli aerosol e la trasmittanza degli strati atmosferici.

Per differenti valori dei raggi delle particelle, delle quote di locazione delle nubi e degli spessori ottici delle stesse, un database spettrale è stato creato.

Il database è il risultato di una procedura di combinazione dei diversi valori assunti dai parametri, precedentemente elencati.

Gli spettri in radianza, ad alta risoluzione, così ottenuti sono stati convoluti sui canali

dello strumento. Al fine di fare il confronto spettrale con i dati delle osservazioni cioè, il segnale è stato degradato alla risoluzione spettrale di VIMS.

Per ogni spettro di VIMS scelto, il best fit con gli spettri sintetici del database fornisce il set di parametri che meglio riproduce il segnale misurato.

Nel calcolo degli spettri sintetici, la geometria osservativa è stata implementata prelevando i valori angolari direttamente dai dati ancillari delle acquisizioni.

Il best fit viene ricavato con una procedura ai minimi quadrati.

Scelta delle immagini

La scelta delle immagini e dei dati spettrali prodotti dallo strumento è stata fortemente condizionata dalla validità delle assunzioni fatte inizialmente sul modello.

Condizioni necessarie al suo corretto funzionamento, come angoli di emissione piccoli e risoluzioni spaziali alte hanno ristretto notevolmente la scelta, unitamente all'esigenza di testare il modello su zone differenti del pianeta.

La scelta ha interessato immagini di orbite diverse, prese in tempi diversi nel corso della missione, anche se va premesso che la sonda è attualmente in orbita e invia costantemente dati verso la Terra.

Questo fatto di per sé impone la scelta dei dati finali per la stesura della tesi come fatto unico ma non esclude in futuro la possibilità di implementazione di dati di maggior interesse.

Fondamentalmente il modello è stato testato in tre regioni ben distinte dell'emisfero sud.

In condizione di estate fino ad agosto 2009, l'emisfero sud ha passato l'equinozio dopo anni di insolazione.

Tre principali regioni dell'emisfero sud sono state considerate per il test del modello: la regione polare, le medie latitudini e la zona equatoriale.

Le osservazioni più rilevanti che sono state implementate fanno riferimento a strutture particolarmente utili ai fini preposti. Si tratta prevalentemente di passaggi, nei quali è possibile vedere condizioni atmosferiche molto diverse.

Ribadiamo come l'invio costante di nuovi dati renda non definitivo il modello.

Risultati

Dal confronto tra i dati osservati e le simulazioni, per la zona polare viene ricavato un valore di particelle piccole ($r_{\text{eff}} = 0.1 \mu m$) che compongono la foschia stratosferica con quote di locazione intorno ai 30 mbar. Per le nubi troposferiche sono ricavati valori di $r_{\text{eff}} = 0.7 \mu m$ con nubilocate a circa 350 mbar. Le nubi profonde, risultano locate a pressioni comprese tra 2 e 4 bar.

Per la regione alle medie latitudini, la foschia stratosferica si trova collocata leggermente più in alto in quota 20 mbar per la regione prima dei 60° con particelle più grandi $r_{\text{eff}} = 0.12 \mu m$. Le nubi troposferiche sono locate più in alto con pressione della base delle nubi a 300 mbar. Quote comprese tra 2 e 3.5 bar sono ricavate per le nubi profonde.

Nel caso equatoriale, il modello non riesce a recuperare il livello del segnale strumentale su tutta la banda passante ma solo nel range tra 2 μm e 4 μm .

Il confronto tuttavia, rivela come tutta la struttura verticale delle nubi sia collocata più in alto.

Per la parte stratosferica vengono ricavati valori delle particelle di $r_{\text{eff}} = 0.2 \mu m$ e pressioni dell'ordine di alcuni *mbar*. Le nubi troposferiche si trovano collocate intorno ai 200 *mbar* con raggi delle particelle che le compongono decisamente più rilevanti ($r_{\text{eff}} = 2 \mu m$).

La procedura adottata non consente al modello l'unicità della soluzione e i parametri ricavati non sono rappresentativi delle reali condizioni osservate ma solo della miglior combinazione dei parametri, fissati *a priori*, che fornisce il miglior fit.

Buona parte dei risultati tuttavia, trova una conferma nella letteratura di argomento, dimostrando come seppur limitato a causa delle forti assunzioni e semplificazioni operate sul modello, quest'ultimo sia in grado di fornire parametri ragionevoli per le strutture atmosferiche osservate e di essere in grado di replicare il livello del segnale misurato dallo strumento.

Alla fine, era la finalità principale del lavoro di tesi.

Instrument and data

Undoubtedly, much of what we know about the Solar System comes from direct exploration.

Since the early 1960's, many robotic spacecrafts have been sent out into our Solar System to explore and return knowledge and images of distant worlds.

With the exception of Pluto¹, all the planets have been visited so far. Some spacecrafts have only flown by some bodies, some have been put into orbit and some have even landed on them.

During this space age, missions of exploration into all the Solar System have revolutionized our view about the nature of it.

Today, we are only at the beginning of this exploration, and even if we have some certain informations, misunderstandings of many physical phenomena involved are still innumerable.

The analysis of all the processes that have shaped our neighboring planets and their moons, and which role these processes may have played in the origin of the Solar System will help us to discover the answers.

Since the invention of the telescope 400 years ago, our ability to measure and analyze the light and its characteristics more and more accurately, has told us very much about what we know, increasing our understanding of the Universe dramatically.

Enormous progress has been made in spectral resolution and in increasing the range of wavelengths over which electromagnetic waves can be measured. Information is acquired detecting and measuring changes that the object causes on the surrounding field (potential, electromagnetic or acoustic). Information acquisition is based on techniques that cover the whole electromagnetic spectrum, from the low-frequency radio waves to the γ -ray regions.

This development has increased our understanding of the formation and evolution of stars and planetary systems.

Space-based observatories have opened up the infrared spectral window, which have allowed the investigation of interstellar clouds as birth-places of stars and the study of circumstellar disks from which it is thought planets may be formed. It is thought that this progress in instrumental techniques continues to flourish, leading possibly to the direct imaging of Earth-like planets, and planets not at all like our own, in the

¹No longer comprised in the Solar System definition however...

not too distant future.

Sensors on satellites orbiting around the Earth provide information about global patterns and dynamics of the atmosphere, surface morphologic structures, ocean surface and wind. The rapid wide coverage capability allows monitoring of rapidly changing phenomena while the long duration and repetitive capability allows the observation of longer term changes. The wide-scale coverage allows the observation and study of regional scale features as well.

Sensors on planetary probes are providing similar information about the planets and objects of the Solar System.

The Cassini-Huygens mission to the Saturnian System means informations acquired by Cassini orbiter's instruments. In this chapter we give a general description of the mission, the instruments involved and the image-spectrometer VIMS in particular, instrument of interest for this research. Most of the technical parts described in the text of next paragraphs are taken from the NASA Cassini mission official documentation [1].

1.1 The Cassini mission

The Cassini mission to Saturn is one of the most ambitious mission in planetary space exploration ever.

Basically it is an enterprise that, from the initial vision to the completion of the mission, will span nearly 30 years.

In 1982 a joint working group was formed by the Space Science Committee of the European Science Foundation and the Space Science Board of the National Academy of Science in the United States. The main goal of the joint was to study possible modes of cooperation between the United States and Europe in the field of planetary science.

European scientists proposed a Saturn orbiter and Titan probe mission to the European Space Agency (ESA), suggesting a collaboration with the U.S. National Aeronautics and Space Administration (NASA).

The mission would be beneficial for the scientific, technological and industrial sectors of all the countries involved.

In 1983, the U.S. Solar System Exploration Committee recommended that NASA include a Titan probe and radar mapper in its core program and also consider a Saturn orbiter.

In 1984-85, a joint NASA/ESA assessment of a Saturn orbiter-Titan probe mission was completed.

In 1986, ESA's Science Program Committee approved Cassini for initial Phase A study, with a conditional start in 1987.

In 1987-88, NASA carried out further work on designing and developing the new spacecraft line. The program was an early effort to reduce the costs of planetary exploration by producing multiple spacecraft for different missions but made with the basic spacecraft components off the same assembly line.

At the same time in Europe, a Titan probe Phase A study was carried out by ESA in collaboration with a European industrial consortium.

In 1989, funding for Cassini was approved by the U.S. Congress. NASA and ESA

simultaneously released announcements of opportunity for scientists to propose scientific investigations for the missions.

ASI² was responsible for different projects of the Cassini spacecraft. The high gain antenna as the visible channel of the image spectrometer on board the orbiter were made by Italian industries.

Cassini was designed to cut the cost of the mission and to simplify the spacecraft and its operation. The design of Cassini is the result of extensive trade off studies which considered cost, mass, reliability, durability, suitability and availability of hardware. To forestall the possibility of mechanical failures, moving parts were eliminated from the spacecraft in favor of instruments fixed to the spacecraft body, whose pointing requires rotation of the entire spacecraft.

The Cassini mission, featuring the intertwined work of NASA, ESA and ASI, have become models for future international space science cooperation.

1.1.1 Flight plane

At 4:43 EST³ on October 15 1997, from Pad 40 at the Cape Canaveral Air Force Station in Florida, a Titan IVB/Centaur launch vehicle is ready to go.

The Cassini's journey begins.

Launch starts with the ignition of the solid rocket motors, which burn for 2 minutes to an altitude of approximately 66 *km*, the Titan's first stage ignites at an altitude of about 58 *km* and at an altitude of approximately 162 *km* the second stage. At approximately 9 minutes into flight at an altitude of about 203 *km*, the Centaur upper stage and the Cassini spacecraft separate from the Titan.

After that the spacecraft and Centaur are injected into a parking orbit around the Earth.

After the Centaur second burn, the Cassini is ready for separation from the mother body. After separating from the Centaur, the control over the spacecraft points the high-gain antenna toward the Sun to ensure the rest of the spacecraft shaded.

During this time Cassini is transmitting real-time telemetry via one of its two low-gain antennas, waiting for instructions...

Flybys

The total mass of the Cassini spacecraft was so large that it was not possible to send it on a direct path to Saturn.

Special maneuvers called "gravity assists" were required to hurl the spacecraft to the target.

After the parking orbit, Cassini used an interplanetary trajectory that took it by Venus twice, then past Earth and Jupiter.

The first two of these four flybys were around Venus, the first one at an altitude of 284 *km* on April 26, 1998, and the second on June 24, 1999, at 600 *km*.

On August 18, 1999, the spacecraft swung past Earth at an altitude of 1.171 *km*. Those three gravity assists were not enough to give Cassini quite as much energy to

²Agenzia Spaziale Italiana. It is the Italian space agency.

³Eastern Standard Time: United States of America official east coast time.

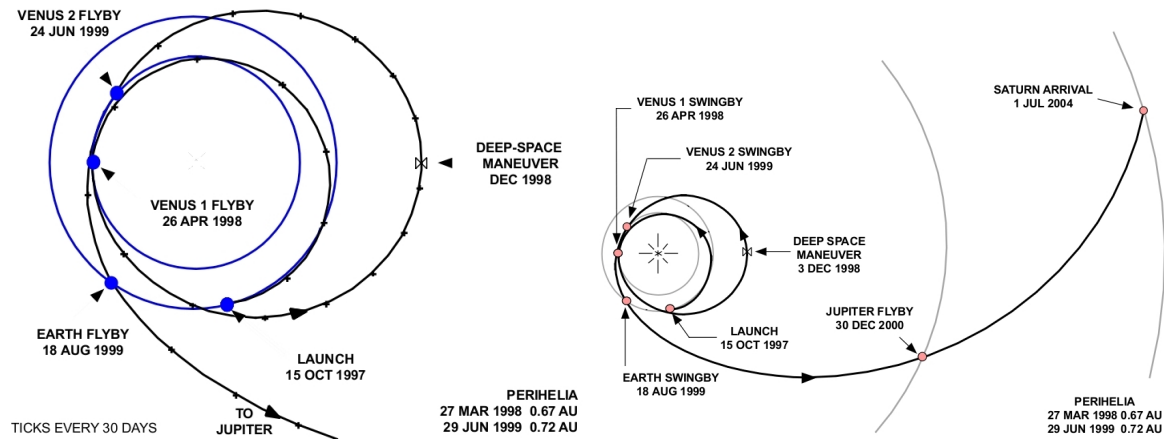


Figure 1.1: *Cassini spacecraft interplanetary trajectory. On the left, the main three gravity assists maneuvers at Venus (twice) and Earth. On the right, the total cruise with the last flyby of Jupiter to the final destination.*

reach Saturn. This is the reason for the need for the fourth and final gravity assist to Jupiter.

Cassini's closest approach to Jupiter was on December 30, 2000, at an altitude of 9.72 million *km*, boosting the spacecraft all the way to Saturn.

This maneuver gave the opportunity to do some science at Jupiter and to study several aspects of its environment from October 2000 through March 2001. During this time, many of the instruments on board the orbiter were turned on for data calibrations, testing and navigation activities as trajectory corrections.

It was a kind of last preparation before the Saturn encounter.

Saturn's orbit insertion

One of the most critical phase of the entire mission.

During the previous seven years, the spacecraft covered about 3.5 billion *km* before encounter the ringed planet.

On the July 1, 2004, Cassini passed through the gap between the F and G Ring.

This maneuver provided a unique opportunity to observe Saturn's Ring and the planet itself, being this the closest approach to Saturn by the spacecraft during the entire mission. The informations gathered on the location and density of material in the Rings was used by orbits designers to plan the most advantageous and safest course for Cassini's flight path. The spacecraft's high-gain antenna was used as a shield to provide maximum protection against any potential dangerous object.

Upon arrival and orbit insertion, Cassini begun its tour of the Saturn system with at least 76 orbits around the planet, including 52 close encounters with seven of Saturn's 31 known moons.

The orbits around Saturn were shaped by gravity-assist flybys of Titan. The size of these orbits, their orientation relative to Saturn and the Sun, and their inclination to

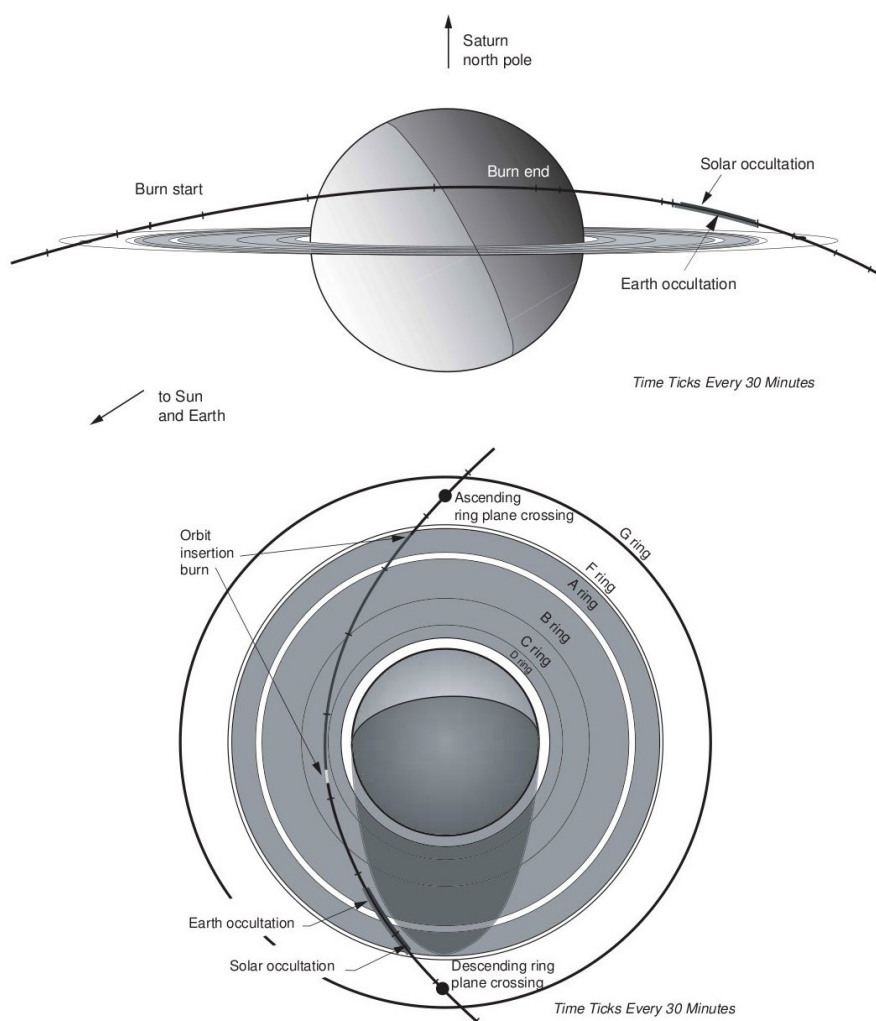


Figure 1.2: *Cassini's arrival geometry at Saturn. The trajectory of the ingress through the Rings's gap is shown.*

Saturn's equator were dictated by various scientific requirements.

In September of the same year, the spacecraft started the maneuver for the second challenge: the landing on Titan's surface.

The Huygens mission

On 25 December, 2004, the Huygens probe has been released from the mother ship, flying on a ballistic trajectory to Titan.

After the release, the Cassini orbiter performed a deflection maneuver after two days. This kept the spacecraft safe from following the probe into Titan atmosphere...

The need for this maneuver was also to establish the required geometry between the probe and the orbiter for radio communications during the probe descent.

The descent of Huygens took place on 14 January, 2005.

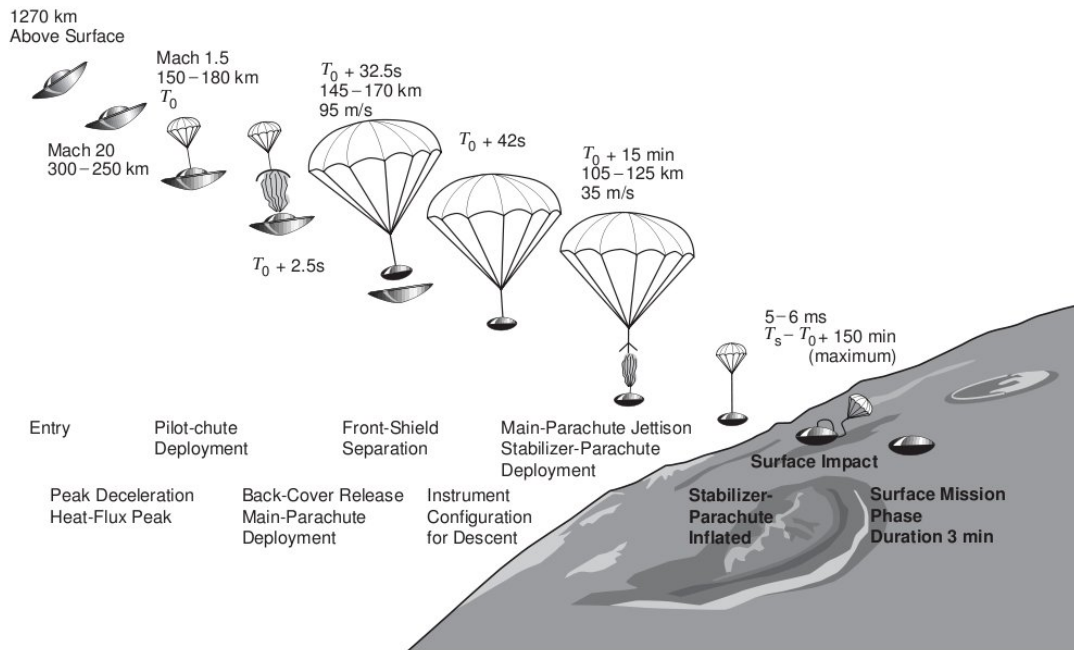


Figure 1.3: *Huygens probe arrival on Titan's surface with the different phases of the descent; from the ingress in the atmosphere to the landing.*

With a speed of almost 22.000 km/h , the probe enter Titan's atmosphere. The Huygens's design is projected to resist the strong change in temperature. From the -200°C of the extreme cold of space to the 1500°C of the intense heat of the bang of the atmospheric entry.

With a help of parachutes the descent was slow to permit the probe to conduct an intensive program of scientific observations all the way down to Titan's surface. When the descent speed had moderated to about 1400 km/h the cover of the probe was pulled off.

After that the main parachute was deployed to ensure the descent stable.

In the final part of the descent, many instruments were turned on to measure the physical properties of the atmosphere. The gas chromatograph and mass spectrometer to determine the chemical composition of the atmosphere as a function of altitude, the aerosol collector and pyrolyzer to capture liquid or solid particles suspended in the atmosphere, heat them and send the resulting vapor to the chromatograph-spectrometer for analysis. More, image and spectral radiometer to take pictures of cloud formations and the surface and also to determine the visibility.

The speed of the impact on the surface was calculated about 25 km/h but one of the most uncertainty was the state of the surface, if solid or liquid, if its landing would have been a thud or a splash!

January 14, 2005, the landing. Huygens is on Titan.

1.1.2 The Spacecraft

The Cassini spacecraft is one of the largest, heaviest and most complex interplanetary spacecraft ever built.

Mainly it is composed by a two part structure: the Cassini orbiter and the Huygens probe.

This last element is deputed to get into the Titan's atmosphere, landing on the planet. The first element of the entire spacecraft is designed to enter in orbit around Saturn, deliver the Huygens probe to its final destination and conduct at least four years of detailed studies of Saturn's system.

Huygens is designed to remain primarily dormant throughout Cassini's journey and then spring into action when it reaches the top of Titan's atmosphere. There, Huygens deploys its parachutes and conduct two and half hour of intensive measurements as it descends through Titan's atmosphere, all the while transmitting its findings to the Cassini orbiter for relay back to Earth.

The weigh of the orbiter alone is 2125 *kg*. With the addition Huygens probe (alone 320 *kg*), a launch vehicle adapter and 3132 *kg* of propellants, the spacecraft reaches a total weight of 5712 *kg*. More than half of the spacecraft's total mass at launch is propellant.

The spacecraft stands 6.8 *m* high and is 4 *m* wide.

The need for protection against the extreme heat and cold of space and in order to maintain the room temperature operating environment needed for computers and other electronic systems on board, most of the spacecraft and its instrument housings are covered with multiple-layered, shiny amber-colored blanketing material.

This kind of materials include layers of mylar to afford protection against micrometeoroids that zip through interplanetary space and which, traveling at speeds of 5 *km/s* to 40 *km/s* , could potentially penetrate portions of the spacecraft.

All the devices are designed to resist the radiation environment of deep space. In particular, when the Sun is at peak activity, its flares, which can last up to several days, can deliver radiation 1.000 times above the usual radiation levels in interplanetary space. All the electronic elements are made to ensure that they won't be disrupted or destroyed by such events.

The mission's trajectory posed a challenge for controlling the spacecraft's temperature in the first several years of the mission because of its proximity to the Sun. During this time, the high-gain antenna was pointed at the Sun and used as a sunshade to shield the rest of the orbiter and probe. Special paints were used on the antenna to reflect and radiate much of the sunlight received. Moving away from the Sun, extreme cold becomes a concern and at Saturn's distance, the intensity of sunlight is approximately only 1 percent of that at Earth.

The complexity of the spacecraft is also demonstrated by the 22.000 wire connections and the 12 *km* of cabling linking its instruments, computers and mechanical devices. The main body of the orbiter is a nearly cylindrical stack consisting of a lower equipment module, a propulsion module and an upper equipment module, and is topped by the fixed 4 meter high-gain antenna. Near the middle of the structure there is a remote sensing pallet, which contains cameras and other remote sensing instruments, and a fields and particles pallet, which contains instruments that study magnetic fields and charged particles.

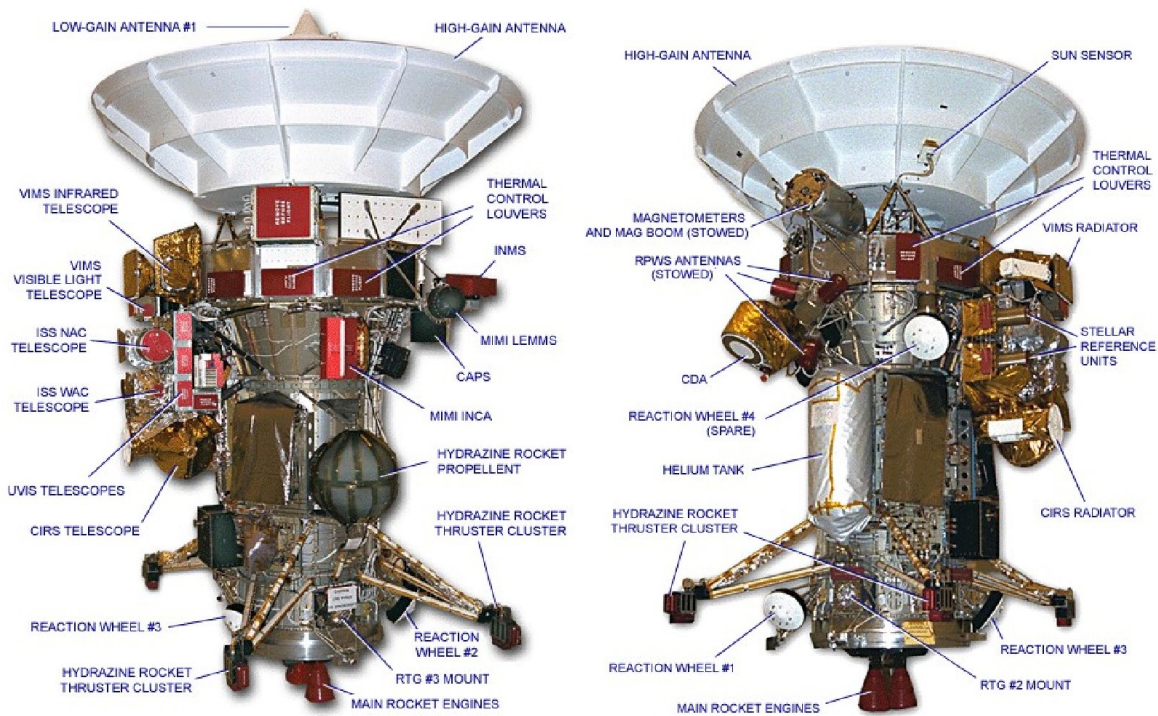


Figure 1.4: Entire spacecraft front-back view. In the left image of the spacecraft is well visible the image spectrometer VIMS allocation.

The two pallets carry most of the Cassini orbiter's science instruments.

In general the whole spacecraft must be turned to point the instruments in the proper direction, though three of the instruments provide their own articulation about one axis.

Software sequences and detailed instructions stored in the spacecraft's computer direct the activities of the spacecraft. A typical sequence may operate Cassini for a month without the need for intervention from ground controllers.

The main source of energy comes from three radioisotope thermoelectric generators. The orbiter receives electrical power from them.

They can produce power by converting heat into electrical energy. The natural radioactive decay of plutonium dioxide is the source of this heat. Devices called thermocouples convert the heat into electricity to run the spacecraft. Similar units were most recently used in other exploration missions, in fact have a long and safe heritage of use and high reliability in NASA's planetary exploration program. Another important aspect of the spacecraft is the control.

Control is governed by sensors that recognize reference stars and the Sun, and by on board computers that determine the spacecraft's orientation. Thanks to new type of gyroscope called an inertial reference unit, the unit can perform turns, twists and propulsion firings while retaining continuous knowledge of its own position.

The Cassini orbiter is a classic stabilized along all three axes spacecraft and thus does not normally rotate during its long cruise to Saturn.

All the communications with the spacecraft during its passage through the inner Solar System were through one of the orbiter's two low-gain antennas. Entering in the

cooler climates of the asteroid belt and beyond in late January 2000 it turned its high-gain antenna toward Earth communicating through it.

In the end, Cassini's cargo of science instruments, the Huygens probe and the amount of propellant the spacecraft carries make it one of the largest interplanetary spacecraft ever launched.

1.1.3 Scientific objectives and payload

Saturn is not a planet. Not only.

It would be better call it system. The Saturn system.

Just like a little Solar System, everything plays its role inside it. The planets itself, the Rings, the moons, a little planet with atmosphere, all the system offers a very rich scientific environment to explore.

The Rings of Saturn are unique in the Solar System in their extent and brightness, maybe they represent the signature feature by which Saturn is known. Very important informations come from the study of the Rings System. It can be considered as a physical model for the disc of gas and dust that surrounded the early Sun and from which all the planets formed.

Measures of the elemental abundance in the atmosphere of Saturn give important informations about constraints on the formation of the Giant Planets. Starting from the expected solar nebula composition is possible to understand how the planets formed. From measures of the gravitational field is possible to understand the shape and the density of the body. Magnetic field data can give us more informations about the electrical currents inside the planet and thus much can be learned about the interior. From wind, temperature, pressure measurements is possible to explain the dynamic of the planet.

The search for other planetary systems depends upon how well we understand the early stages of formation of planets. Detailed knowledge of the history and processes now occurring on Saturn's elaborately different moons may provide valuable data to help understand how each of the Solar System's planets evolved to their present states.

One of the main scientific goals within of Cassini mission is the unmasking of Titan. Titan is the only moon in the Solar System that possesses a dense atmosphere (1.5 times denser than Earth's). Its atmosphere is rich in organic material and the fact that living organisms as we know them are composed of organic⁴ material is particularly intriguing.

The importance of Titan's atmosphere and the Huygens mission dedicated to it, is related to the role that organic material can plays in life's beginning. Many experiments in the modern age, are still seeking fundamental clues to the question of how life began on Earth. Life could be the final result of combinations of complex carbon compounds in a primeval soup. Anyway, one of the main problem in this kind of investigations is the ignorance about the chemical circumstances on the young Earth. What we need to know is which starting material was present at the beginning of life on Earth. More, only Earth and Titan have atmospheres rich in nitrogen, hydrocar-

⁴Here "organic" means only that the material is carbon based and does not necessarily imply any connection to living organisms.

bonds like the methane present on Titan may have been abundant on the young Earth. The importance of Titan in this connection is that it may preserve, in deep-freeze, many of the chemical compounds that preceded life on Earth. Some scientists believe we will find that Titan more closely resembles the early Earth than Earth itself does today.

The Cassini and Huygens mission main science objectives can be summarized as follows:

Saturn

- Determine the temperature field, cloud properties and composition of Saturn's atmosphere.
- Measure the planet's global wind field, including waves and eddies; make long term observations of cloud features to see how they grow, evolve and dissipate.
- Determine the internal structure and rotation of the deep atmosphere.
- Study daily variations and relationship between the ionosphere and the planet's magnetic field.
- Determine the composition, heat flux and radiation environment present during Saturn's formation and evolution.
- Investigate sources and nature of Saturn's lightning.

Titan

- Determine the relative amounts of different components of the atmosphere; determine the mostly likely scenarios for the formation and evolution of Titan and its atmosphere.
- Observe vertical and horizontal distributions of trace gases; search for complex organic molecules; investigate energy sources for atmospheric chemistry; determine the effects of sunlight on chemicals in the stratosphere; study formation and composition of aerosols (particles suspended in the atmosphere).
- Measure winds and global temperatures; investigate cloud physics, general circulation and seasonal effects in Titan's atmosphere; search for lightning.
- Determine the physical state, topography and composition of Titan's surface; characterize its internal structure.
- Investigate Titan's upper atmosphere, its ionization and its role as a source of neutral and ionized material for the magnetosphere of Saturn.

Magnetosphere

- Determine the configuration of Saturn's magnetic field, which is nearly symmetrical with Saturn's rotational axis. Also study its relation to the modulation of Saturn kilometric radiation a radio emission from Saturn that is believed to be linked to the way electrons in the solar wind interact with the magnetic field at Saturn's poles.

- Determine the current systems, composition, sources and concentrations of electrons and protons in the magnetosphere.
- Characterize the structure of the magnetosphere and its interactions with the solar wind, Saturn's moons and Rings.
- Study how Titan interacts with the solar wind and with the ionized gases within Saturn's magnetosphere.

The Rings

- Study configuration of the Rings and dynamic processes responsible for Rings structure.
- Map the composition and size distribution of Rings material.
- Investigate the interrelation of Saturn's Rings and moons, including embedded moons.
- Determine the distribution of dust and meteoroid distribution in the vicinity of the Rings.
- Study the interactions between the Rings and Saturn's magnetosphere, ionosphere and atmosphere.

Icy Moons

- Determine general characteristics and geological histories of Saturn's moons.
- Define the different physical processes that have created the surfaces, crusts or subsurfaces of the moons.
- Investigate compositions and distributions of surface materials, particularly dark, organic rich materials and condensed ices with low melting points.
- Determine the bulk compositions and internal structures of the moons.
- Investigate interactions of the moons with Saturn's magnetosphere and Rings System and possible gas injections into the magnetosphere.

In addition to the science objectives at Saturn, the Cassini spacecraft will also conduct a gravitational wave search through the ASI-provided high-gain antenna during its interplanetary cruise.

Payload

The Cassini orbiter and the Huygens probe were equipped with a set of high technical instruments and devices able to collect different data informations and spectra from the visible light to the infrared. An array of eighteen instruments are mounted on board the entire spacecraft, twelve for the orbiter and six for the lander.

All the equipment covers different scientific areas and research fields. The instruments are mainly involved in optical remote sensing, fields, particles and waves measurements, microwave remote sensing and imaging.

We can summarize the complete payload for the entire spacecraft as:

Cassini orbiter instruments

Visible and Infrared Mapping Spectrometer (VIMS): Imaging grating spectrometer designed to measure reflected and emitted radiation, is able to map the surface spatial distribution of the mineral and chemical features of a number of targets, including Saturn's Rings, surfaces of the moons, and the atmospheres of Saturn and Titan. The instrument includes two different spectrometers that split the light received from objects into its component wavelengths. The instrument obtains information over 352 contiguous wavelengths from $0.35\ \mu\text{m}$ to $5.1\ \mu\text{m}$; it measures intensities of individual wavelengths and use the data to infer the composition and other properties of the object that emitted the light. The mapping function of the instrument will provide images in which every pixel contains high-resolution spectra of the corresponding spot on the target body.

Composite Infrared Spectrometer (CIRS): Dual interferometer that measures infrared emissions from atmospheres, Rings and surfaces within the Saturn system. This spectrometer creates vertical profiles of temperature and gas composition for the atmospheres of Titan and Saturn, from deep in their tropospheres (lower atmospheres), to high in their stratospheres (middle atmospheres). The instrument will also gather information on the thermal properties and composition of Saturn's Rings and icy moons. The instrument is a coordinated set of three interferometers designed to measure infrared emissions from $1400\ \text{cm}^{-1}$ to $10\ \text{cm}^{-1}$ over wavenumber grid (from $7\ \mu\text{m}$ to $10^3\ \mu\text{m}$ in wavelengths units) in the mid- and far-infrared range of the electromagnetic spectrum. Each interferometer uses a beam splitter to divide incoming infrared light into two paths. The beam splitter reflects half of the energy toward a moving mirror and transmits half to a fixed mirror. The light is recombined at the detector. As the mirror moves, different wavelengths of light alternately cancel and reinforce each other in a pattern, called an interferogram, that depends on their wavelengths and intensities. This information can be used to determine the infrared spectrum.

Imaging Science Subsystem (ISS): Cassini's cameras, will photograph a wide variety of targets: Saturn, the Rings, Titan and the icy moons, from a broad range of observing distances for various scientific purposes. General science objectives include studying the atmospheres of Saturn and Titan, the Rings of Saturn and their interactions with the planet's moons and the surface characteristics of the moons, including Titan. The instrument includes both a wide-angle camera ($60.0\ \mu\text{rad}/\text{pixel}$ angular resolution) and narrow-angle one ($6.0\ \mu\text{rad}/\text{pixel}$ angular resolution). The narrow-angle camera provides high-resolution images of targets of interest, while the wide-angle camera provides more extended spatial coverage at lower resolution. The cameras can also obtain optical navigation frames images of Saturn's moons against a star background which are used to keep the spacecraft on the correct trajectory.

Ultraviolet Imaging Spectrograph (UVIS): Basically is a set of detectors designed to measure ultraviolet light reflected by or emitted from atmospheres,

Rings and surfaces to determine their compositions, distributions, aerosol content and temperatures. The instrument will also measure fluctuations of sunlight and starlight as the Sun and stars move behind the Rings of Saturn and the atmospheres of Saturn and Titan, and will determine the atmospheric concentrations of hydrogen and deuterium. The instrument includes a two-channel, far- and extreme-ultraviolet imaging spectrograph that studies light over wavelengths from 55.8 *nm* to 190 *nm*. It also has a hydrogen deuterium absorption cell and a high-speed photometer. An imaging spectrograph records spectral intensity information in one or more wavelengths of light and then outputs digital data that can be displayed in a visual form. The hydrogen-deuterium absorption cell will measure the quantity of deuterium, a heavier form (isotope) of hydrogen. Hydrogen-deuterium ratio varies widely throughout the Solar System and is an important piece of data in understanding planetary evolution. The high-speed photometer determines the radial structure of Saturn's Rings by watching starlight that passes through the Rings.

Cassini Plasma Spectrometer (CAPS): Measures the composition, density, flow velocity and temperature of ions and electrons in Saturn's magnetosphere. The instrument consists of three sensors: an electron spectrometer, an ion beam spectrometer and an ion mass spectrometer. A motor-driven actuator rotates the sensor package to provide 208° scanning in the azimuth of the Cassini orbiter. The electron spectrometer makes measurements of the energy of incoming electrons; its energy range is 0.7 to 30 *keV*. The ion beam spectrometer determines the energy to charge ratio of an ion; its energy range is 1 electron volt to 50 kilo-electron volts. The ion mass spectrometer's energy range is 1 *eV* to 50 *keV*. The instrument measures the flux of ions as a function of mass per charge, and the flux of ions and electrons as a function of energy per charge and angle of impact relative to the instrument itself.

Cosmic Dust Analyzer (CDA): It is able to provide direct observations of small ice or dust particles in the Saturn system in order to investigate their physical, chemical and dynamic properties and study their interactions with the Rings, icy moons and magnetosphere of Saturn. The instrument measures the amount, velocity, charge, mass and composition of tiny dust and ice particles. It has two types of sensors high-rate detectors and a dust analyzer. The two high-rate detectors, intended primarily for measurements in Saturn's Rings, count impacts up to 10⁴ particle/*s*. The dust analyzer will determine the electric charge carried by dust particles, the flight direction and impact speed, mass and chemical composition, at rates up to one particle/*s*, and for speeds of up to 100 *km/s*. An articulation mechanism allows the entire instrument to be rotated or repositioned relative to the body of the Cassini orbiter.

Ion and Neutral Mass Spectrometer (INMS): It is intended to determine the composition and structure of positive ions and neutral particles in the upper atmosphere of Titan and the magnetosphere of Saturn, and will measure the positive ion and neutral environments of Saturn's icy moons and Rings. The instrument will determine the chemical, elemental and isotopic composition of the gaseous and volatile components of the neutral particles and the low energy

ions in Titan's atmosphere and ionosphere, Saturn's magnetosphere and the Ring environment.

Dual Technique Magnetometer (MAG): Primary objective is to determine the planetary magnetic fields and the dynamic interactions in the planetary environment and analyze Saturn's magnetic field and interactions with the solar wind. The instrument consists of direct sensing instruments that detect and measure the strength of magnetic fields in the vicinity of the spacecraft. The experiment includes both a flux gate magnetometer and a vector/scalar helium magnetometer. They are used to measure the magnitude and direction of magnetic fields. Since magnetometers are sensitive to electric currents and ferrous metal components, they are generally placed on an extended boom, as far from the spacecraft as possible. On Cassini, the flux gate magnetometer is located midway out on the 11 *m* magnetometer boom, and the vector/scalar helium magnetometer is located at the end of the boom. The boom itself, composed of thin, nonmetallic rods, was folded during launch and deployed about two years after launch. The magnetometer electronics are located in a bay in the Cassini orbiter's spacecraft body.

Magnetospheric Imaging Instrument (MIMI): Designed to measure the composition, charge state and energy distribution of energetic ions and electrons; detect fast neutral particles; and conduct remote imaging of Saturn's magnetosphere. It is the first instrument ever designed to produce an image of a planetary magnetosphere. This information will be used to study the overall configuration and dynamics of the magnetosphere and its interactions with the solar wind, Saturn's atmosphere, Titan, Rings and the icy moons. The instrument will provide images of the ionized gases, called plasma, surrounding Saturn and determine the charge and composition of ions. Like the Cassini plasma spectrometer, this instrument has three sensors that perform various measurements: the low-energy magnetospheric measurement system, the charge-energy-mass spectrometer and the ion and neutral camera. The low-energy magnetospheric measurement system will measure low- and high-energy proton, ion and electron angular distributions (the number of particles coming from each direction). The charge-energy-mass spectrometer uses an electrostatic analyzer, a time-of-flight mass spectrometer and microchannel plate detectors to measure the charge and composition of ions. The third sensor, the ion and neutral camera, makes two different types of measurements. It will obtain three-dimensional distributions, velocities and the rough composition of magnetospheric and interplanetary ions.

Radio and Plasma Wave Science (RPWS): The main functions are to measure electrical and magnetic fields in the plasma of the interplanetary medium and Saturn's magnetosphere, as well as electron density and temperature. Plasma is essentially a soup of free electrons and positively charged ions, the latter being atoms that have lost one or more electrons. Plasma makes up most of the Universe and is created by the heating of gases by stars and other bodies in space. Plasma is distributed by the solar wind; it is also "contained" by magnetic fields of bodies such as Saturn and Titan. The major components of the instrument are an electric field sensor, a magnetic search coil assembly and a

Langmuir probe. The electric field sensor is made up of three deployable antenna elements mounted on the upper equipment module of the Cassini orbiter. Each element is a collapsible beryllium-copper tube that was rolled up during launch and subsequently unrolled to its approximately 10 *m* length by a motor drive. The magnetic search coils are mounted on a small platform attached to a support for Cassini's high-gain antenna. The Langmuir probe, which measures electron density and temperature, is a metallic sphere about 50 *mm* in diameter. The probe is attached to the same platform by an approximately 1 *m* deployable boom.

Radio Science Subsystem (RSS): This set of devices use the spacecraft's radio and the ground antennas of NASA's Deep Space Network to study the composition, pressures and temperatures of the atmospheres and ionospheres of Saturn and Titan; the radial structure of and particle size distribution in Saturn's Rings; and the masses of objects in the Saturn system and the mass of Saturn's Rings System as a whole. Radio science will also be used to search for gravitational waves coming from beyond our Solar System. Some of these experiments measure Doppler shifts (frequency shifts) and other changes to radio signals that occur when the spacecraft passes behind planets, moons, atmospheres or physical features such as planetary Rings. From these measurements, information about the structures and compositions of the occulting bodies, atmospheres and Rings can be derived. RSS is split in two parts: one resides on the spacecraft, the other at stations equipped to receive very stable radio signals.

Radio Detection and Ranging Instrument (RADAR): It uses the five-beam Ku-band antenna feed assembly associated with the spacecraft high gain antenna to direct radar transmissions toward targets, and to capture blackbody radiation and reflected radar signals from targets. It investigates the surface of Saturn's largest moon, Titan. The instrument is based on the same imaging radar technology used in missions such as the Magellan mission to Venus and the Earth-orbiting Spaceborne Imaging Radar. Investigations about the geological features and topography of Titan's solid surface are planned. The radar takes four types of observations: imaging, altimetry, backscatter and radiometry. In imaging mode, the instrument will bounce pulses of microwave energy off the surface of Titan from different incidence angles and record the time it takes the pulses to return to the spacecraft. These measurements, converted to distances by dividing by the speed of light, will allow construction of visual images of the target surface with a resolution ranging from about 0.3 *km* to 1.7 *km*. Radar altimetry similarly involves bouncing microwave pulses off the surface of the target body and measuring the time it takes the "echo" to return to the spacecraft. In this case, however, the goal will not be to create visual images but rather to obtain numerical data on the precise altitude of surface features. The altimeter resolution is about 24 *km* to 27 *km* horizontally, and 90 *m* to 150 *m* vertically. In backscatter mode, the radar will bounce pulses off Titan's surface and measure the intensity of the energy returning. This returning energy, or backscatter, is always less than the original pulse, because surface features reflect the pulse in more than one direction. Conclusions about the

composition and roughness of the surface from the backscatter measurements can be derived. In radiometry mode, the radar will operate as a passive instrument, simply recording the heat energy emanating from the surface of Titan. This information will be used to determine the amount of heat absorption by gases and aerosols, a factor that has an impact on the accuracy of the other measurements taken by the instrument. The radar will be used in different ways at different altitudes. At altitudes between about 22.5 *km* to 9 *km*, the radar will switch between scattering measurements and radiometry in order to obtain low-resolution global maps of Titan's surface roughness, backscatter intensity and thermal emissions. At altitudes between about 9 *km* to 4 *km*, the instrument will switch between altimetry and radiometry, collecting surface altitude and thermal emission measurements. Below about 4 *km*, the radar will switch between imaging and radiometry.

Huygens probe instruments

Descent Imager and Spectral Radiometer (DISR): Is uses 13 fields of view, operating at wavelengths of 350 *nm* to 1700 *nm*, to obtain a variety of imaging and spectral observations. Infrared and visible imagers will observe Titan's surface during the latter stages of the descent. By taking advantage of the Huygens probe's rotation, the imagers will build a mosaic of pictures around the landing site. A side-looking visible imager will view the horizon and the underside of any cloud deck. Solar aureole sensors will measure the light intensity around the Sun resulting from scattering by particles suspended in the atmosphere, permitting calculations of their size, number and density.

Huygens Atmospheric Structure Instrument (HASI): Investigates the physical properties of Titan's atmosphere, including temperature, pressure and atmospheric density as a function of altitude, wind gusts and wave motion ⁵. Comprising a variety of sensors, the instrument will also measure the ion and electron conductivity of the atmosphere and search for electromagnetic wave activity. On Titan's surface, the instrument will be able to measure the conductivity of surface material. The instrument also processes the signal from the Huygens probe's radar altimeter to obtain information on surface topography, roughness and electrical properties.

Aerosol Collector and Pyrolyzer (ACP): This instrument traps particles suspended in Titan's atmosphere using a deployable sampling device. Samples will be heated to vaporize the ice particles and decompose the complex organic materials into their component chemicals. The products will then be passed to the gas chromatograph/mass spectrometer for analysis. The instrument will obtain samples at two altitude ranges. The first sample will be taken at altitudes down to about 30 *km* above the surface. The second sample will be obtained at an altitude of about 20 *km*.

Gas Chromatograph and Spectrometer (GCMS): It is able to provide a quantitative analysis of Titan's atmosphere. Atmospheric samples will be trans-

⁵This last option was in the event of a landing on a liquid surface only.

ferred into the instrument by dynamic pressure as the Huygens probe descends through the atmosphere. The mass spectrometer will construct a spectrum of the molecular masses of the gas sampled by the instrument. Just before landing, the instrument's inlet port will be heated to vaporize material on contact with the surface. Following a safe landing, the instrument will be able to determine Titan's surface composition. The mass spectrometer serves as the detector for the gas chromatograph, for atmospheric samples and for samples provided by the aerosol collector and pyrolyzer.

Doppler Wind Experiment (DWE): Using two ultrastable oscillators, one on the Huygens probe and one on the Cassini orbiter, it is able to give Huygens' radio relay link a stable carrier frequency. Orbiter measurements of changes in probe frequency caused by Doppler shift will provide information on the probe's motion. An height profile of wind and its turbulence can be derived.

Surface Science Package (SSP): This device contains a number of sensors to determine the physical properties and composition of Titan's surface. An acoustic sounder measures the rate of descent, surface roughness and the speed of sound in any liquid. During descent, measurements of the speed of sound give information on atmospheric composition and temperature. An accelerometer records the deceleration profile at impact, indicating the hardness of the surface. Tilt sensors (liquid-filled tubes with electrodes) measure any pendulum motion of the Huygens probe during descent, indicate the Huygens probe orientation after landing and measure any wave motion. A group of platinum resistance wires, through which a heating current can be passed, will measure temperature and thermal conductivity of the surface and lower atmosphere and the heat capacity of the surface material. The instrument will also provide some crude topographic mapping of the surface as the probe descends the last few meters through the atmosphere.

Once the spacecraft's on board recording device reaches capacity, it points its high-gain antenna toward Earth and downloads the data through one of the 70 *m* antennas of the Deep Space Network ⁶. Italian contribution provides Cassini with the core of the telecommunication system: the High-Gain Antenna (HGA). At the top of the Cassini stack is the large, 4 meter diameter HGA and two low-gain antennas (LGA1 and LGA2). HGA is also used for radio and radar experiments and it was used for receiving signals from Huygens. The two microwave remote-sensing experiments, RADAR and RSS, share the spacecraft's HGA.

In the end, Cassini's payload represents a carefully chosen set of interrelating instruments that address many major scientific questions about the Saturn system. The data they return are analyzed by a team of nearly 300 scientists from the United States and Europe.

⁶Communications with Cassini during the mission are carried out through those NASA's stations. They're located in California, Spain and Australia. Data from the Huygens probe have been received and relayed by the network and sent to the European Space Agency operations complex in Darmstadt, Germany.

1.2 Visible Infrared Mapping Spectrometer

VIMS is a remote sensing instrument designed, built and developed for the Cassini mission to Saturn by an international team representing the national space agencies of different countries.

The first imaging spectrometer designed for planetary exploration was NIMS⁷, assembled by JPL⁸ in the late 1970's for the Galileo mission to Jupiter. In the subsequent years, the american agency studied many ways to improve the technology and produced designs for other planetary applications [47].

The primary purpose of the instrument is to provide two dimensional high resolution multispectral images which are able to study the composition of the materials of the surface of Saturn's satellites, its atmosphere, the structure of the atmosphere and the surface of Titan, the nature of the Rings and more.

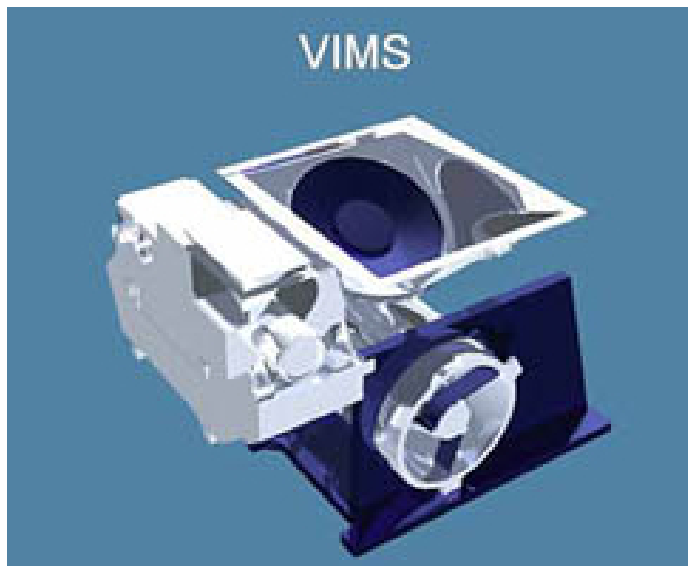


Figure 1.5: 3D image of VIMS. Basically is a dual image spectrometer. The visible and infrared channels are side by side.

The instrument's unique system design consists of two different spectrometers actually: VIMS-V for the visible part of the electromagnetic spectrum and VIMS-IR for the near infrared part, covering a total wavelength range from $0.35 \mu m$ to $5.1 \mu m$ with 352 channels.

The two optical systems are boresighted and operate in tandem, coordinated by a common electronic units.

The term "mapping" is referred to a particular operating mode of the instrument.

Normal spectrometers can operate in mapping mode by moving the telescope to position the entrance slit over different parts of the target object but on the Cassini orbiter this would mean moving the entire spacecraft to point the instrument.

The ability of VIMS is to move its primary mirror to obtain spectral informations of

⁷Near Infrared Mapping Spectrometer. It was the image spectrometer of the Galileo mission to Jupiter.

⁸Jet Propulsion Laboratory - Pasadena California (USA). American space agency specialized in planetary mission

the target without repositions of the spacecraft.

That's why VIMS is called "mapping" image spectrometer.

Next a general description of the two channels is given and how they work together to give the scientific data we use for this work.

1.2.1 VIMS-V image spectrometer

The visible channel of VIMS is one of the most important contributions of ASI to the Cassini mission.

The instrument covers the wavelength range from $0.3\ \mu\text{m}$ to $1.05\ \mu\text{m}$, through 96 channels. The optical head is electrically coupled to an electronics box.

The optical system consists of a $f/3.2$ off-axis telecentric *Shafer* telescope, an *Offner* grating and a calibration unit. The *Shafer* configuration is an *Offner* relay adapted to an inverted *Burch* telescope.

In this configuration the telescope, consisting of two concentric spherical mirrors, is corrected for spherical aberration, coma and astigmatism but it has a curved field and an obscured secondary mirror that is larger than the primary.

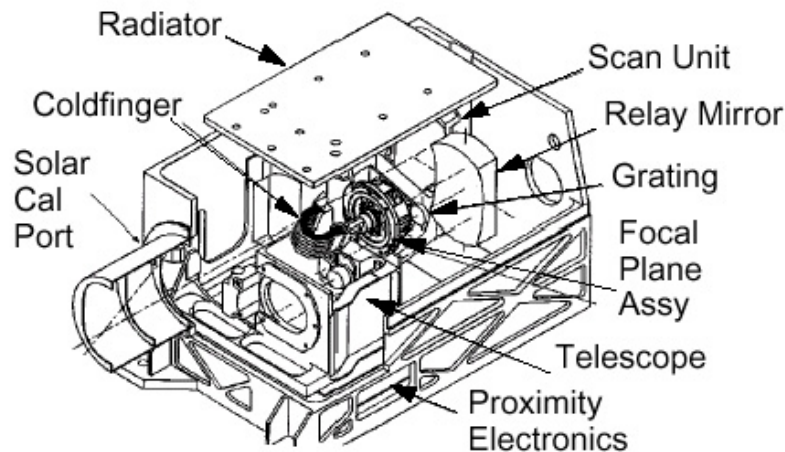


Figure 1.6: Open scheme of the visible channel VIMS-V Optical Head. The position of the single components inside the box is also shown.

If the telescope is inverted as in *Shafer's* idea, the primary is larger than secondary and the anastigmatic features remains, albeit the image is virtual and behind the secondary. An *Offner* relay, consisting of two off-axis concentric spheres operating as unit magnification, is able to provide a real image on a flat, distortion-free field [39]. All the optical design utilizes the symmetrical principle to have maximum benefit. When the elements of any optical system are made symmetrical, coma and distortion can be almost completely eliminated over an appreciable field. In the VIMS-V case, both the spectrometer and the telescope incorporate *Offner* relays that are not only symmetrical conjugates of each other, which enables further aberration compensation and stray light reduction, but they are each symmetrical within themselves [39]. All but two mirrors of the system are square cut-outs, this in order to reduce the total mass and volume of the system.

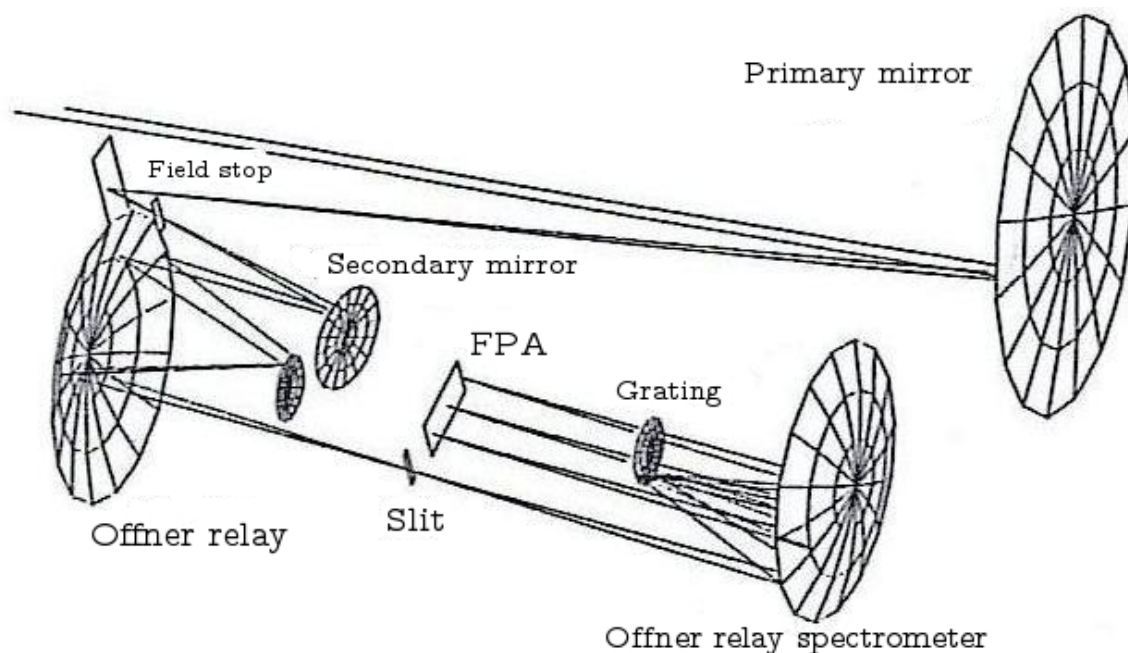


Figure 1.7: *VIMS-V optical system raytrace. From the primary mirror the light goes to the secondary mirror through the field stop and then to the Offner relay. After the slit another Offner relay reflects the light to the grating for dispersion on the FPA.*

Quasi-collimated light enters at 0° (or within the $\pm 1.2^\circ$ scan angles) and reflects off the decentered concave primary mirror onto the tilted folding flat. The flat redirects the converging beam through the first field stop to the convex spherical secondary. From this point, the light enters the *Offner* relay by reflecting off the large concave spherical mirror onto the convex spherical secondary, which is the aperture stop. From the stop mirror the beam reflects back onto the large relay mirror before exiting through the imaging slit to the spectrometer.

To make all the system telecentric, it was necessary to put the pupil at a distance of 68 cm from the primary mirror. Placing an aperture stop at the center of curvature of a spherical mirror makes the system monocentric, that's why the position of the aperture stop is so important.

VIMS-V aperture stop is located on the *Offner* secondary, which is sufficiently close to the "effective center of curvature" to reduce aberrations. The image slit however, is very near the center of curvature of the final spherical mirror and limits coma and astigmatism in the spectral direction.

The diffraction grating manufactured by *Carl Zeiss* factory, is convex and holographically recorded in a Rowland circle configuration.

The groove profile is rectangular from a laminar construction and the spacings of the grooves are equidistant. The efficiency of the grating varies as a function of the depths of the grooves. The diffracted beam returns to the relay mirror before it ventures toward the detector plane.

The Focal Plane Assembly (FPA), receive the dispersed light coming from the grat-

ing. The FPA is composed by a CCD⁹, manufactured by *Loral*, this is a front side illuminated frame transfer NMOS device with a buried channel design, having a 512×256 sensible elements matrix.

Many modern spacecrafts use this device to take informations from a target. Usually is an integrated circuit having a two-dimensional array of hundreds of thousands or millions of charge-isolated wells, each representing a pixel. Light falling on a well is absorbed by a photoconductive substrate such as silicon releasing a quantity of electrons proportional to the intensity of light incoming. the electronics of the device detects and stores accumulated electrical charge representing the light level on each well over time. An image can be so reconstructed pixel by pixel from each level at different wavelengths.

All the flying instruments need to be re-calibrated after the shock of the launch, the sleep of the long journey and/or other eventualities. The radiometric transfer function obtained during the on-ground calibration is not sufficient to remove instrumental effects when applied to in-flight data. Since it is no possible for the instruments to point at a target on the spacecraft, each instrument must provide its own calibration source.

VIMS-V uses two LED¹⁰ with widely separated peak wavelengths, on the red and the green, to check the spectral dispersion end relative efficiency of the spectrometer. It uses the Sun, which is the source for all visible channel measurements, to archive direct and absolute radiometric calibration before data collection.

The scan mirror is rotated to an optical angle of 4.0° to view the red and green light emissions coming from a beam splitter (used in reverse mode) and two lenses that spread the beam it traverses a prism system that directs the beam at the correct angle toward the primary mirror.

The pair of LED are also used to check the angle accuracy of the scan unit's resolver. Another calibration source is the solar one, where the spacecraft must position itself so that the port is 20° from the boresight. The Sun light passes through the solar port, a rectangular cut-out entrance, at the same angle of the Sun.

1.2.2 VIMS-IR image spectrometer

The optical design of the infrared channel of VIMS comes directly from the NIMS experience [44].

Working on 256 bands between $0.85 \mu m$ e $5.1 \mu m$, VIMS-IR is an evolution of NIMS project and even if the design is drawn from the Galileo mission instrument, new important differences vastly improve VIMS-IR performance over NIMS.

Most of the infrared channel structure, optics and passive radiative cooler is actually a renewed flight-quality prototype for the NIMS system. Other differences with NIMS are the two-scan mechanism for the telescope secondary mirror that replaces the single-axis NIMS mirror scanner, the shutter mechanism that was developed to replace the chopper mechanism, a new radiator shield [38].

The telescope of the optical system consist of a 23 cm diameter $f/3.5$ *Richey-Chretien* with a scanning secondary mirror coupled to a triple-blaze grating spectrometer with

⁹Charge-Coupled Device

¹⁰Light Emitting Diode

an $f/3.5$ Dahl-Kirkham collimator and an $f/1.86$ flat field camera.

The FPA of VIMS-IR, developed by *Cincinnati Electronics* under the JPL authority, is a linear array of 256 InSb (Indium Antimonide) photodetectors which are read simultaneously by a pair of multiplexers. Inside the IR channel, a passive radiative cooler is used to cool the FPA to its operating temperature. All the package is designed to interface to the cooler, which keeps the FPA within the 60 K to 77 K temperature range.

Inside the package and directly over the detector array, a set of four order sorting filters are precisely mounted to prevent higher order spectra and out-of-band radiation from contaminating the narrow band light to be measured by each detector. Each of them is $200\ \mu\text{m} \times 103\ \mu\text{m}$ in size, with $123\ \mu\text{m}$ between detector centers.

The multiplexers are arranged on either side of the array and each one is configured to read the odd or even numbered detectors respectively¹¹. the signal from each multiplexer is read out by the electronic ensuring a degree of redundancy.

If one multiplexer or its downstream signal processing fails in fact, the data from the other multiplexer still could provide limited coverage over the full spectral range.

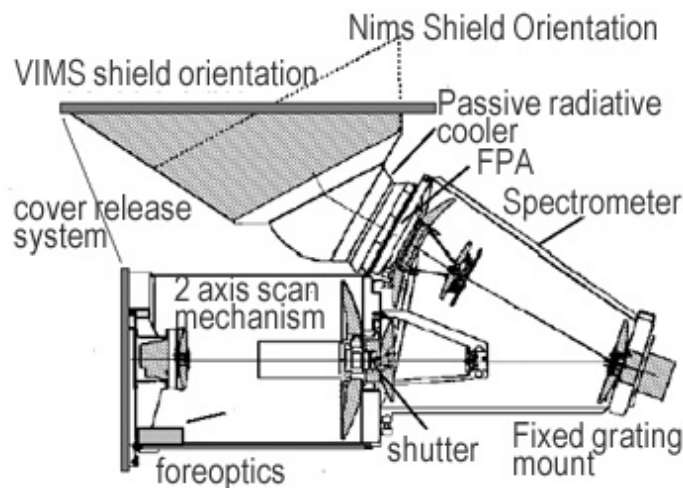


Figure 1.8: VIMS-IR 2D lateral section. The dotted line shows the different orientation of the shield of NIMS.

To provide in-flight calibration of spectral performance a port for viewing the Sun was incorporated not only for the visible channel but for infrared as well. The Sun is an ideal calibration source because its spectrum is well known over the VIMS spectral range and bandwidths and because the Sun is the external light source for VIMS imaging.

Also, since the Cassini UVIS instrument point a special port at the Sun as part of its experiment, regular opportunities for Sun acquisition are available.

For VIMS-IR however, the problems posed by a solar port were how to adequately attenuate the light to within the dynamical range of the FPA in a spectrally repeatable manner and how to utilize the full optical path of the instrument.

¹¹The multiplexer on one side reads the odd detectors and the even ones are read by the other multiplexer.

	VIS channel	IR channel	Total system
Spectral range	0.30 – 1.05 μm	0.85 – 5.1 μm	0.30 – 5.1 μm
Spectral resolution	High res = 1.46 nm/spectel Nom res = 7.3 nm/spectel	16.6 nm/spectel	
Spectral bands	96	256	352
Inst. field of view (IFOV)	0.17 $\times$ 0.17 mrad	0.25 $\times$ 0.50 mrad	
Effective IFOV (=1 pixel)	3 $\times$ 3 sum	1 $\times$ 2 on-chip sum	0.5 $\times$ 0.5 mrad
Field of view (FOV)	64 pixel (1.83°) X-axis 64 pixel (1.83°) Z-axis	64 pixel (1.83°) Z-axis 64 pixel (1.83°) X-axis	64 pixel (1.83°) X-axis 64 pixel (1.83°) Z-axis
Swath width	576 IFOV (3 $\times$ 3 $\times$ 64)	128 IFOV	64 pixel X-axis
Image size variability	1, 12, 32, 64 pixels ²	1, 12, 32, 64 pixels ²	1, 12, 32, 64 pixels ²
Image scan motion	64 lines on Z-axis	128 IFOVs in X-axis	64 lines in Z-axis
Channels boresights coalignment			$\leq$ 1 pixel
Spectral registration			$\leq$ 1 pixel
Effective focal length	143 mm	426 mm	
f -number	$f/3.2$	$f/1.86$	
$A\Omega$	$4.42 \cdot 10^{-7} \text{ cm}^2 \text{ ster}$	$4.37 \cdot 10^{-5} \text{ cm}^2 \text{ ster}$	
Geometric throughput	100%	55%	
Spectrometer grating type	Holographic	Plane	
Entrance slit width	20 $\mu m \times 6 \text{ mm}$	0.2 $\times$ 2.4 mm	
Grating blazes	2 laminar depths	3 ruled angles	
Grating groove density	349.8 grooves/mm	36.2 grooves/mm	
Internal spectral calibration	2 LEDs	1 Laser diode	
External spectral calibration	Solar port	Solar port	
Radiometric calibration	Stars, planets	Stars, planets	
Dark signal calibration	Space background	Closed shutter	
Detector type	Si-CCD 512 $\times$ 256 pixels	InSb 256 pixels	
Active area	24 $\times$ 24 μm /pixel	103 $\times$ 200 μm /pixel	
Quantum efficiency	$0.13 \leq Q \leq 0.41$	$Q \geq 0.70$	
Max charge storage	$3 \cdot 10^5 \text{ eV}$, $9 \cdot 10^5 \text{ eH}$	$2.5 \cdot 10^6 \text{ e}$	
Readout noise	10 $e \cdot rms$	$\leq 500 \text{ e}$	
Dark current	40 pA/cm ² at 22 °C	3 pA/cm ² at 64 K	
Digitalization	12 bits	12 bits	12 bits
Pixel integration times	80 ms to 130 s	13 ms to 12 s	
System peak power			23.9 W
Telemetry output data rate			183 kbit/s
Data compression			> 2–1
Detector operating temperature	-40 °C to -20 °C	-213 °C to -196 °C	
Optics operating temperature	-10 °C to +20 °C	-143 °C to -113 °C	
Electronics operating temperature	-20 °C to +50 °C	-20 °C to +50 °C	-20 °C to +50 °C

Table 1.1: *VIMS design specifications for the visible and infrared channels and for the total instrument* [18]

We said that the solar calibration port takes light incident at an angle of 20 ° from the main aperture boresight in the direction of the Cassini high gain antenna. While the look angle of the calibration port is fixed with respect to the spacecraft, its field of view is the same as the instrument to allow compensation of possible spacecraft pointing errors.

The VIMS-IR internal calibration source is a Laser diode that plays the same role of the LED in the VIMS-V instrument. The diode, placed inside the port, can be used to check for shifts in spectral registration at times when solar disk is not in the field of regard.

1.2.3 Instrument data acquisition

VIMS-V and VIMS-IR are different for many technical aspects but they work in unison to provide data set that appears as if it were made by a single device.

VIMS can be operated in a variety of modes determinate by several parameters. The parameters of image size and integration time most directly determine the data rate. Due to their different detector configuration however, precise synchronization of their mirror motion and data collection is critical.

Because the visible channel uses an area array CCD detector, it acquires its data in "push-broom" mode. It views one row of a square scene at time only. This row is imaged as one row of pixels on the CCD and the spectrometer spectrally disperses the image of this row so that each row of the CCD views the image in a different waveband contiguous with its neighboring rows.

To acquire a square image the CCD is read after each row is acquired and the mirror moves to the next row in the scene.

The infrared channel uses a linear array detector so it acquires its data in "whiskbroom" mode, where it views a single spatial pixel per exposure only.

The spectrometer disperses the image of this pixel on the FPA so that each detector views the pixel in a different contiguous waveband. To provide synchronous data with the VIMS-V, VIMS-V must sweep its single pixel field of view along the identical row in the scene that the VIMS-V is observing within the same exposure time.

To create a two dimensional image. the two channels begin at the top of the desired scene and acquire data row by row. This requires perfect synchronization and excellent geometric alignment.

To obtain the final image of a scene in all the waveband of the instrument, each channel must synthesize a square nominal system pixel of $(0.5 \times 0.5) \text{ mrad}$, by summing more than one exposure of their detectors. The pixel summing and image scanning process however, is further complicated because the two channels have different detector sizes [38].

VIMS-V pixel are $(0.167 \times 0.167) \text{ mrad}$ squares so a 3×3 grid of the optical head pixels is summed to equal one system pixel. To sum 3 IFOV in one dimension the optical head steps its mirror twice while continuously integrating during a single exposure time. Then the electronics commands the CCD to sum every three pixels in the other dimension upon transfer to its horizontal register. This results in an equivalent 0.5 mrad square IFOV pixel. Five pixels are also summed in the spectral dimension to achieve the 7.3 nm specified nominal visible spectral bandwidth.

VIMS-IR has rectangular detectors so during the time it is imaging a single square IFOV it is continuously integrating while its mirror moves over two of its actually rectangular IFOV to obtain the $(0.5 \times 0.5) \text{ mrad}$ nominal system pixel. Because the two-axis scan mechanism of the secondary mirror, this last one is driven for each axis in uniform steps.

Data is collected only during the X-axis scan motion, which then flies back to the next Y-axis starting position in preparation for the next line. All the pixel summing and image process is illustrated in Figure 1.9.

VIMS can also operate in other modes for specialized investigations.

We mention the "point" mode, where measures spectra at a single pint in the space, useful for occultation studies where stars spectra are tracked in the deep space or behind an atmosphere, and the "line" mode where measures a single line in space which is useful for fast object flybys.

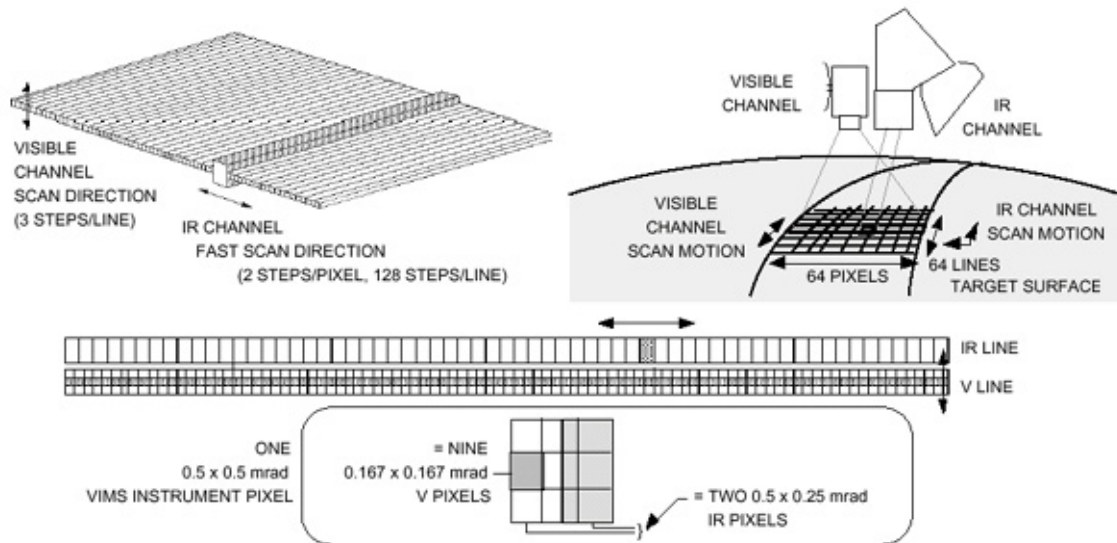


Figure 1.9: *VIMS total pixels synthesis and image operations. Starting from their different IFOV, VIMS-V acquires an entire line at the same time, while VIMS-IR sums all the 64 pixels to get the line.*

1.3 The Cubes

The previous description explains the instrument in general and how it acquires data. We have seen that in order to obtain the two dimensional images of either low or high spatial resolution, each channel of VIMS uses a scanning mirror. At each position of the scanning mirror the light of the spatial elements within the slit is spectrally dispersed by the grating in 352 spectral bands.

The final result is a data set called "Cube".

The "Qubes" files are used for storing multi-dimensional data arrays. The maximum number of supported dimensions is six. A "Cube" file is a special case of a qube file in which the number of dimensions in the data array is three.

The VIMS data cubes follow the PDS¹² international protocol for the planetary data. A PDS labeled file consists of two basic parts. The first part is the label, which is located at the beginning of the file. The remainder of the file is the data area which contains one or more data object. The label describes the structure and content of the file and the informations are stored in a "keyword=value" text format. Typical informations can be the number and the name of the axis, their length, the spectral band covered and more. In the PDS protocol files without label inside can also exist. Three main different configuration are possible: Attached, where the label with the informations is inside the file, Detached: where the label is in a separated file connected to the data file through a pointer and Combined Detached: where there is only one separated label for different files. Cube files are normally used for storing data produced by imaging spectrometers. Thus, two of the dimensions correspond to spatial coordinates and the other dimension corresponds to the spectral coordinates.

¹²Planetary Data System. PDS is an archive of data products from NASA planetary missions, which has become a basic resource for scientists around the world. <http://pds.jpl.nasa.gov/>.

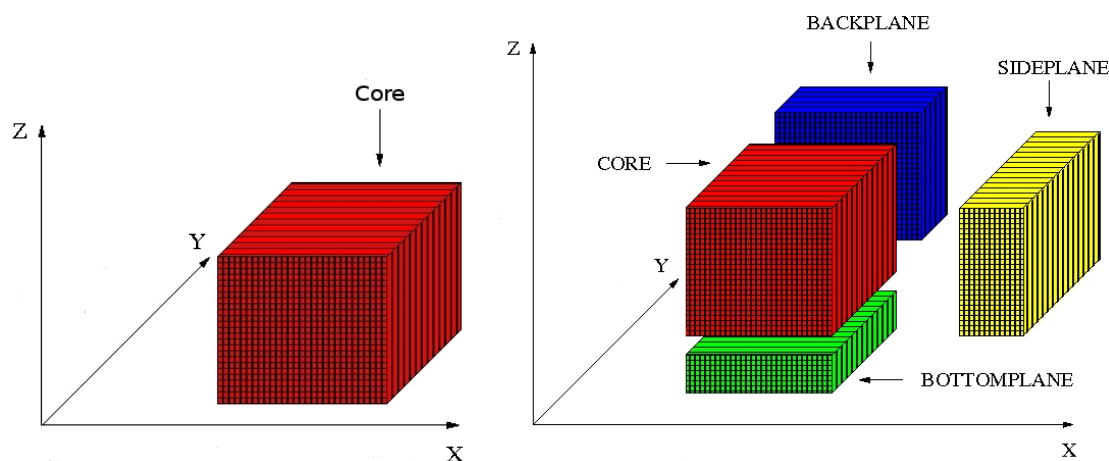


Figure 1.10: Graphics example of a generic image spectrometer data cube object. On the left the data core array, where the main physical informations are stored. On the right, the core complete of its suffix planes extension, where typically engineering data are stored in. The X-axis is related to the sample, the Z-axis to the lines and the Y-axis to the bands.

The two spatial dimensions correspond to the line and the sample. The visible channel primary mirror scan direction (as the infrared channel slow scan direction as well) is on the line-axis, while the infrared channel fast scan direction is on the sample-axis. The contents of the data values in a standard cube file can of course consist of things other than observations measured by an imaging spectrometer.

The name cube is absolutely without any real physical meaning. It is only an informatic architecture, a conceptual or "logical" view of the data itself.

The main informations are stored in the "core" of the structure. The core region of the cube data object contains the main data array that is being stored inside. Being VIMS an image spectrometer, the core consists of a number of spatial image planes corresponding to a different wavelength bands. Each of the three axis in a cube data object however, may optionally include suffix data that extend the length of the axis. Conceptually, this can be viewed as forming one or more suffix planes that are attached to the core cube. Suffix planes that extend the samples dimension are called SIDEPLANES, suffix planes that extend the lines dimension are called BOTTOMPLANES and suffix planes that extend the bands dimension are called BACKPLANES. The suffix planes are used for storing auxiliary data that are associated with the core data, many ancillary data or engineering informations can be stored inside the planes.

Most application programs provide this logical view of a cube to a user but we remark that this view is separate from the issue of the physical storage of the data object in a file.

From an informatic point of view the file in which a cube data object is stored is physically accessed as if it were a one-dimensional data structure. storing the cube pictured above thus requires that the logical three-dimensional structure be mapped into the one-dimensional physical structure.

This involves moving through the three-dimensional structure in certain patterns to

determine the linear sequence of core and suffix planes that occur in the file. This pattern is defined specifying which axis index varies fastest in the linear sequence of values in the file, which varies second fastest and which varies slowest. The typical cube-processing that programs support are three:

- BSQ - Band Sequential (SAMPLE, LINE, BAND)
- BIL - Band Interleaved by Line (SAMPLE, BAND, LINE)
- BIP - Band Interleaved by Pixel (BAND, SAMPLE, LINE)

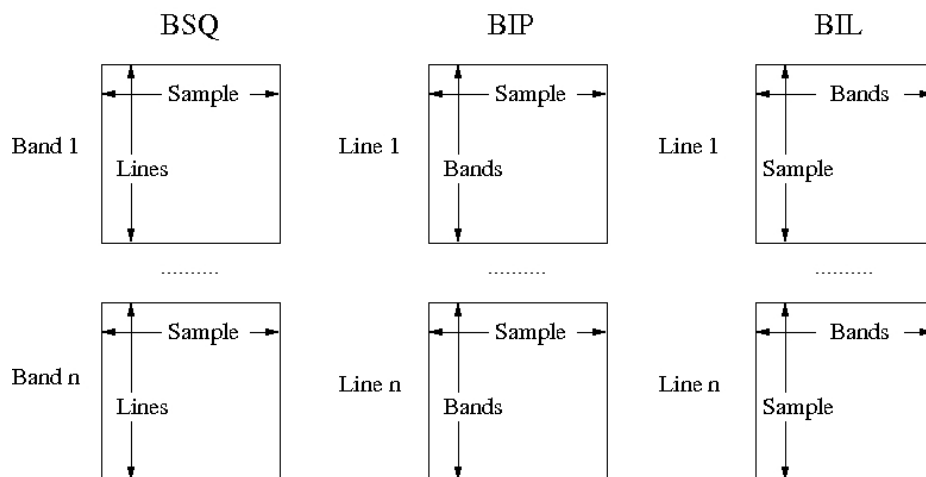


Figure 1.11: *The three main cube processing formats. the Band sequential is most used. The program read the pixel as first object and then the line, for every single wavelength band.*

The order of these values corresponds to the order of the readed axes. For example, in a BSQ storage order file, the physical cube storage in the file begins with the pixels in the first line of the spatial image plane at the first wavelength band. This is followed by the sideplane values that extend this line of core values. Next are the core pixels for the second line, followed by the sideplane values for the second line and so on. After the last line of this first core image plane come the bottomplane pixels associated with the first band. This is then repeated for the second through last bands. Finally, all the backplane are stored after all the core data and associated sideplane and bottomplane.

We mention the fact that if a cube file includes suffix planes on more than one axis, then the region that is the intersection between two (or all three) of the suffix regions is called a CORNER region. Space for corner region data are allocated in the cube files but these data are currently not used by any application programs.

To have an idea of the instrument's data, in Figure 1.12 examples of acquisitions are shown. The images of Saturn are taken near the end of the cruise phase of the Cassini's journey. The planet is well visible in all its entire shape.

The images show Saturn both in visible and infrared bands (upper figure).

The visible RGB image on the left has been made at wavelengths $\lambda_R = 702.9 \text{ nm}$,

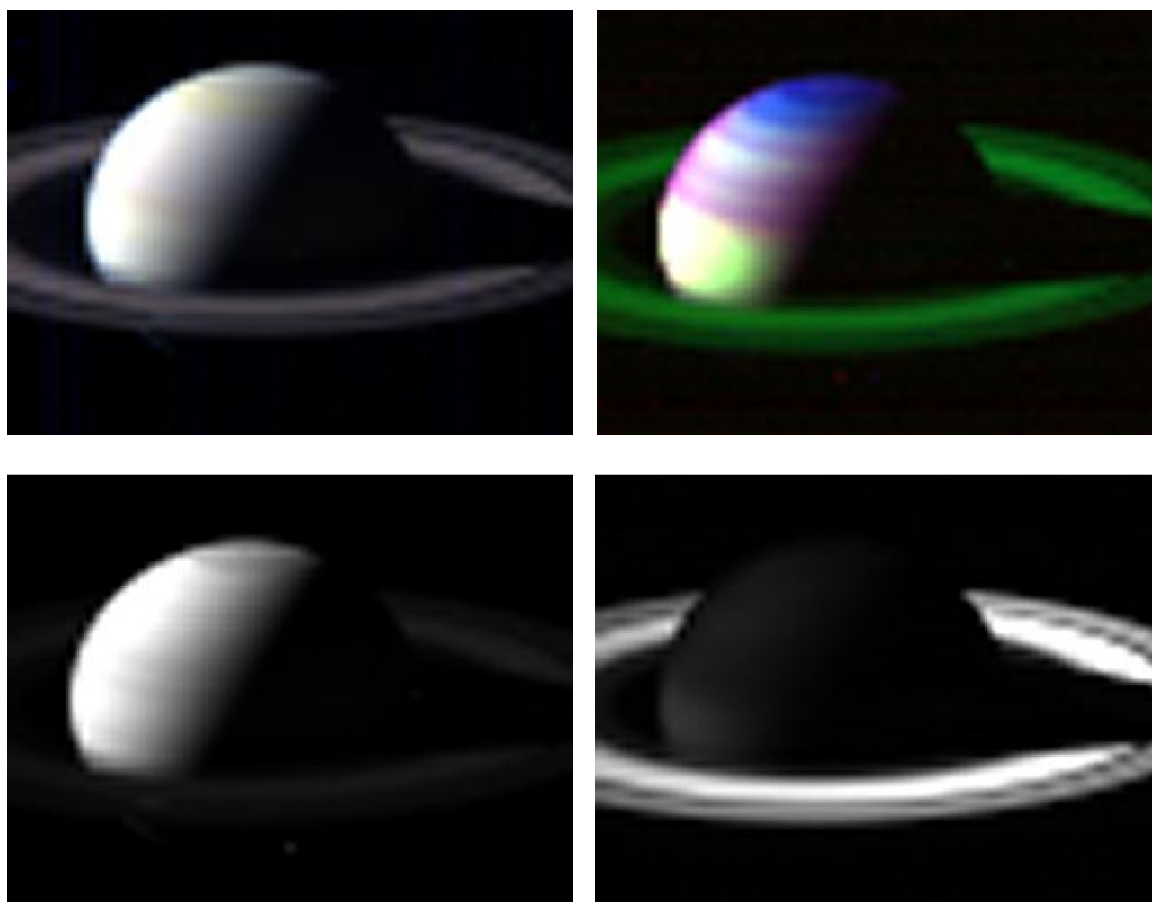


Figure 1.12: In the upper two figures, Saturn both in visible (left) and infrared (right) RGB bands. Below, monochromatic gray scale pictures of the planet at two different wavelengths (see text for explanations).

$\lambda_G = 549.5 \text{ nm}$ and $\lambda_B = 439.2 \text{ nm}$, for the infrared RGB image we have used $\lambda_R = 4515.9 \text{ nm}$, $\lambda_G = 2516.6 \text{ nm}$ e $\lambda_B = 1524.2 \text{ nm}$.

In the others two figures below there's an example of the 'gray scale' mode for the infrared channel only. The image on the left has been taken at $\lambda = 1524.2 \text{ nm}$, at that wavelength there is a spectral window in the Saturn's atmosphere spectrum and so it is possible to see the whole planet while the Rings made mainly of water ice, disappear because that element absorbs at that wavelength.

The image on the right is the same but at $\lambda = 1393.2 \text{ nm}$, in this case the opposite effect is predominant. The atmosphere absorbs and the Rings reflect the light making the planet disappear.

For all the procedures and analysis of the VIMS data we have used the ENVI/IDL¹³ package software. It is a very complex and useful software in order to handle the image-spectrometers data, which permits many mathematical processing and graphics elaborations.

¹³Acronym for Enviroment for the Visualization of Images / Interactive Data Language. www.itt.com

Radiative Transfer Processes

Most of the scientific investigations are directly or indirectly based on the electromagnetic field and its properties.

Many instruments read informations from the electromagnetic waves producing other informations in many ways. The electromagnetic field is very often the driver of many physical *principia* and it can be considered as a "gods's messenger" not only for the atmospheric science but for many other disciplines as well.

The exploration of far worlds is probably the classic example.

Every time the instrument-target distances became big enough to make the direct contact impossible, the electromagnetic field is the only possibility to get informations.

Remote Sensing technique, is the capability to get informations trough the radiation emitted by a target without any direct contact.

In this chapter, some of the molecular spectroscopic theoretical concepts will be shown, useful to understand most of the work done. Some of the fundamental relations and formulas of radiative transfer are discussed also.

By the way, *remote sensing* does not mean space exploration only.

We perceive our surrounding world through our five senses; sight and hearing do not require close contact between sensors and externals, thus our eyes and ears are remote sensors.

We perform *remote sensing* essentially all of the time...

2.1 Notions of molecular spectroscopy

Spectroscopy is an extremely powerful tool in the study of atoms and molecules.

It is well known that when photons hit atoms or molecules of a chemical element in their fundamental state, the electrons jump on orbitals with different energies. These internal molecular energies are all quantized and can be separated into electronic, vibrational and rotational.

There are significant differences between the energies involved in the various regions of the electromagnetic spectrum. The first type of energy is typically associated with the absorption or the emission in the visible part of the electromagnetic spectrum, the vibrational and rotational are typical of the infrared and microwave regions, re-

spectively.

A molecule consisting of two (or more) nuclei is held together by valence binding forces of electrons and balanced by internal repulsion forces. The molecule is in ground state when the outer electronic configuration is in equilibrium and has potential energy in electronic form when the configuration is unstable due to acquisition of energy either via absorption or collision.

Since the internuclear spacing is large compared to the diameters of the nuclei, which act as point masses, the molecule possesses moments of inertia about certain axes and can therefore rotate about them.

Small changes in energy levels can produce changes in kinetic energy of rotation and thus angular velocity of rotation. The valence bond holding the nuclei together is not rigid, thus it can be stretched and compressed slightly, creating changes in intermolecular distance. This elastic bond allows the nuclei to vibrate about their equilibrium positions; however transitions between vibrational energy levels require much more energy than those of rotation. Even more energy is needed for the energy change associated with electronic arrangement.

Vibration and rotation do not occur separately in nature however and observed spectra show both types of transitions simultaneously in their line structure. The vibration-rotation combination gives rise to a rotational fine structure around each vibrational line.

The quantum mechanic explained the quantized energy states available to an electron in orbit about a nucleus. Additional consideration of elliptical orbits, relativistic effects, and magnetic spin orbit interaction was needed to explain the observed emission spectra in more detail, including the fine structure observed. Explanation of molecular emission lines is still more complicated. Gaseous emission spectra are found to have atomic spectral lines with many additional molecular emission lines superimposed.

The spectra structure is due to the state of the matter and three major types of molecular excitation are observed:

- *line spectra*: it is a discrete sequence of separated spectral lines at different frequencies and represents the electronic excitation when the orbital states of the electrons change in the individual atoms.
- *band spectra*: the lines are condensed in a specific region of frequencies, forming bands separated each other. Represents the vibrational excitation when the individual atoms vibrate with respect to the combined molecular center of mass.
- *continuous spectra*: many frequencies in a relatively wide spectral region. The rotational excitation when the molecule rotates about the center of mass.

Each transition involving a change in electron energy produces a whole series of emission or absorption lines, since many combinations of changes in vibration and rotation energy are possible. If such a system of lines is observed under low resolution conditions, it appears to be a band with practically a continuous distribution of frequencies. The spectrum of a molecule is therefore composed of a set of bands due to vibrational state changes, along with a fine structure of lines in each vibrational band due to changes in the rotational state.

Radiation-matter interaction

Two types of processes can be classified: extinction and emission of radiation.

Extinction can be divided into absorption and scattering.

One basic type of interaction between radiation and matter can be summarized by a photon transferring all of its energy to an atom or a molecule and thus being removed from the radiation field.

The energy of the photon raises an electron to a higher energy level or a molecule to higher rotational or vibrational states. This increase in energy of the receiving atom or molecule can be released in several different ways.

One mechanism is for the activated molecule to collide with another molecule, and to drop back into a lower energy state; the energy thus freed becomes kinetic energy of the molecules and corresponds to warming the gas. The photon is permanently lost or attenuated from the radiation field.

This is absorption.

A second mechanism for release of the energy increase is the spontaneous transition of the molecule into its original state by emitting a photon which is identical to the absorbed one except for its direction of propagation. In this case, the photon remains part of the radiation field but the direct beam is attenuated.

This is scattering.

The subdivision depends on the physical process involved, in particular changes of internal or kinetic energy of the particle. For an elastic scattering process the energy of the incident and scattered photon is the same, no energy is transformed to the scattering particle in form of kinetic or internal energy. Else, the scattering process is inelastic and called absorption.

As the matter of interest is basically molecules, exhibiting electronic, vibrational, and rotational internal levels of energy, any change to a higher energetic state is commonly also called absorption.

If the absorbed photon, however, is re-emitted, there is no conversion to translational, i.e. kinetic and hence thermal energy. Considering the total energy, then the process is one of pure scattering. The difference in the usage of the term absorption has to be kept in mind and the meaning should be clear from the context. When the question is about planetary energy budget and heating of an atmosphere, the conversion into thermal energy is of interest.

For the method of absorption spectroscopy on the other hand, only the loss of a photon from its initial path is of importance.

Electronic, vibrational, and translational energy levels can be excited by the absorption of a photon, if its energy equals the difference of two molecular energy levels. The transition probability shows a linear dependence on the energy density of the radiation field and is obtained from quantum mechanical calculations. Before an absorbed photon is re-emitted, it is possible that non-radiating transitions take place due to molecular collisions. The energy of the photon is then transferred to kinetic energy.

A third mechanism is the activated molecule releases its energy spontaneously but in two different stages.

Two photons with different lower energies result; the sum of the energies of the two photons equals the energy of the absorbed photon. The direct beam is attenuated;

the original photon has been replaced by two photons at longer wavelengths and is no longer part of the radiation field. This is *Raman scattering*.

We mention other mechanisms for energy release as fluorescence and phosphorescence. These occur when the energy is not released spontaneously, but after relaxation times of nanoseconds to hours.

Another basic type of interaction involves the conversion of molecular kinetic energy (thermal energy) into electromagnetic energy (photons). This occurs when molecules are activated by collisions with each other and the activation energy is emitted as photons.

This is emission and occurs simultaneously with absorption.

2.1.1 Spectral line width

If a spectrometer was infinitely perfect, the absorption process of a photon by an atom would show an infinitely narrow feature, a zero width line centered at only one absolute frequency.

For the real instruments, a line is not monochromatic and always appears spread over a finite wavenumber range with a definite and reproducible line shape. The instrumentation used for observing a spectrum in fact, is itself one of the major limiting factor in the observed line shape.

But not only.

There are several factors, other than instrumental ones, which contribute to the observed line shapes. Different physical processes are involved in the absorption and emission of radiation by atoms or molecules, all contributing to the lines spread. The most important are the *Natural line broadening*, related to quantum effects and the *Pressure broadening* and *Doppler broadening*, more related to the physical state of the gas.

The main parameters that identified a line are the central frequency ν_0 where the absorption or emission occurs, the line intensity S and the shape or profile, a normalized mathematical function $\Phi(\nu - \nu_0)$.

Natural line broadening

According to Heisenberg's Uncertainty Principle, the Natural line broadening arises from the finite lifetime Δt of spontaneous decay transitions.

It is a phenomenon of quantum mechanical nature and implies that the energy levels are not precisely defined but have a spread of values ΔE . This indetermination is reflected to the times and the frequencies through the famous relation:

$$\Delta E \Delta t = \hbar \quad (2.1)$$

where $\hbar = h/2\pi$ with h Planck's constant and being $\Delta t \propto (2\pi\Delta\nu)^{-1}$, to each transition is associated a range of frequencies with a certain probability of interacting with the molecule.

line broadening due to the natural line width is small relative to most other contributions but is contributed to in an identical way by each atom or molecule and so is

an example of homogeneous broadening.

The natural line broadening is much larger at visible and ultraviolet wavelengths than at infrared wavelengths and is usually much smaller than the broadening seen in planetary spectra. The broadening of lines due to the loss of energy in emission (natural broadening) is practically negligible as compared with that caused by collisions and the Doppler effect.

Pressure (or Collision) broadening

The second reason of the line width is due to the inevitable interactions between atoms or molecules.

This broadening arises from the fact that collisions between molecules, during a spontaneous state transition, diminish the natural lifetime of the transition Δt to the mean time between collisions.

If τ is the mean time between collisions in a gaseous sample and each collision results in a transition between two different states there is a line broadening $\Delta\nu$, coming from:

$$\Delta\nu = (2\pi\tau)^{-1} \quad (2.2)$$

The relation between pressure and line shape was obtained by Lorentz and has become known as the *Lorentian line shape*:

$$\Phi_L(\nu - \nu_0) = \frac{\alpha_L/\pi}{(\nu - \nu_0)^2 + \alpha_L^2} \quad (2.3)$$

where α_L is the HWHM ¹ that, if we use the kinetic gases theory, is equal to:

$$\alpha_L = \alpha_{L_0} \frac{p}{p_0} \sqrt{\frac{T_0}{T}} \quad (2.4)$$

where $p_0 = 1000 \text{ mb}$, $T_0 = 273 \text{ K}$ and α_{L_0} is the HWHM value at temperature and pressure standard conditions². In predicting the line shape due to collisions. Lorentz assumed that, on collision, the oscillation in the atom or molecule is halted and, after collision, starts again with a phase completely unrelated to that before collision.

Because α_L is proportional to the pressure and being the expression normalized, for high values of pressure, the contribution of the wings of the function become important.

We mention other two important aspects of the HWHM: α_{self} and α_{air} .

The first one is due to the effect of the pressure of a molecule by all the other molecules of the same specie, the second is due to all the other molecules in the gas. If a specie is only in trace in the atmosphere, the first one is often negligible.

¹Half Width at Half Maximum.

²The temperature ratio in the α_{L_0} expression has an exponent $n = 0.5$, this number determining the temperature dependence is called the *line width exponent*. For most optically active gases, $0.6 < n < 0.8$. This range can differ considerably for different molecules. This discrepancy arises because the optical cross section of the molecules have a temperature dependence.

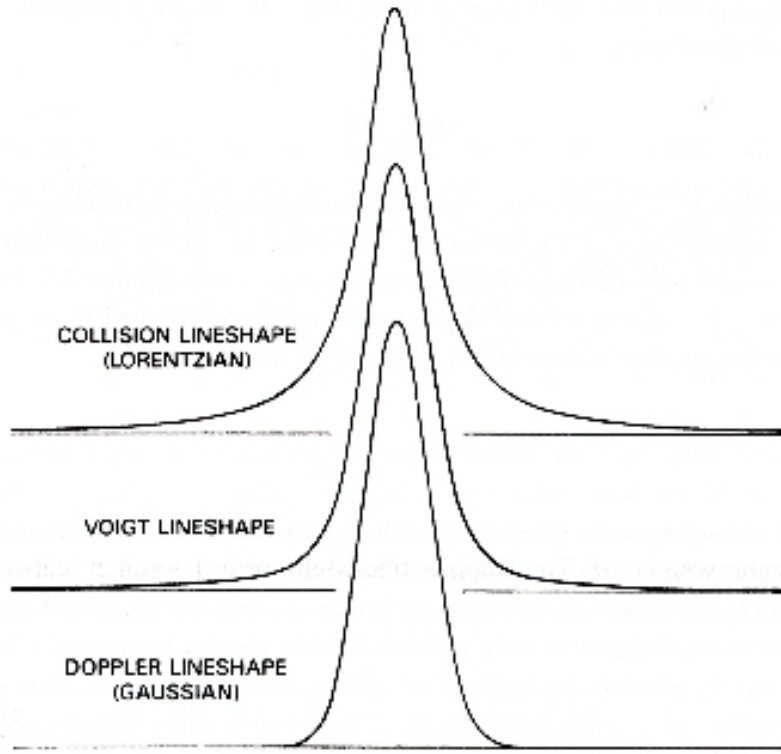


Figure 2.1: *Voigt line profile compared with a Lorentz and Doppler line profiles. All three profiles have the same maximum and half width amplitude for an easy comparison.*

Doppler broadening

It well known that the relative motion between an observer and an emitting source produces the *Doppler effect*.

In a similar way the frequency of a train's whistle increases as the train travels with constant velocity towards an observer and decreases as it leave the observer, the frequency of the radiation absorbed during a transition in an atom or molecule differs according to the direction of motion relative to the source of radiation. The shape of the Doppler line is given by:

$$\Phi_D(\nu) = \frac{1}{\sqrt{\pi}\alpha_D} e^{-(\nu-\nu_0)^2/\alpha_D^2} \quad (2.5)$$

with

$$\alpha_D = \frac{\nu_0 v_0}{c} \quad v_0 = \sqrt{\frac{2k_B T}{m}} \quad (2.6)$$

where ν_0 is the frequency of the photon³, v_0 is the velocity obtained from the Maxwell distribution and m is the mass.

If for the Pressure broadening the pressure is responsible for the line width, in this

³In quantum mechanic is a quantum of energy and defined as $E = h\nu$

case is the temperature. Being α_D proportional to the temperature in fact, heavy molecules give low broadening and *vice versa*.

Voigt line shape

When the pressure broadening and the thermal broadening occur together and no one of them is negligible, they contribute both to the line spectra. The composite line profile, which must now include the effects of both, is obtained from the convolution of the two profiles. Voigt line broadening has no analytical expression but can be computed numerically. The Voigt line shape approaches the Lorentz line shape at high pressures and the Doppler line shape at low pressures.

Skipping all the calculations, the final expression of the shape is:

$$\Phi_V(\nu) = \frac{r_{L/D}}{\sqrt{\pi^3} \alpha_D} \int_{-\infty}^{+\infty} \frac{e^{-y^2} dy}{(v - y)^2 + r_{L/D}^2} \quad (2.7)$$

where $r_{L/D} = \alpha_L/\alpha_D$, $v = (\nu - \nu_0)/\alpha_D$ and $y = v_x/v_0$ with v_x velocity of the particle along the x axis. The expression $\Phi_V(\nu)$ is called *Voigt profile* and if normalized, describes both the Natural-Pressure and Doppler broadenings. In particular:

- for $r_{L/D} \rightarrow 0$ gives Doppler profile
- for $r_{L/D} \gg 1$ follows Lorentzian profile;
- for values of $r_{L/D}$ between the two previous ones shows a Doppler shape like near the center of the line and a Lorentz shape like on the wings.

The Voigt line has no analytical expression but can be computed numerically.

Once the line shape $\Phi(\nu)$ is known however, in order to obtain a complete spectral information we have to consider the product of the lineshape and the intensity of the absorption or emission process:

$$\sigma(\nu) = S \Phi(\nu - \nu_0) \quad (2.8)$$

where S is defined as the *line strength* expressed in m^2/s units.

2.1.2 Absorption coefficient

In general spectral lines are assumed to be symmetric about the central frequency, which corresponds to a maximum absorbing power. In the case of a symmetric line, well separated from neighbouring lines of the absorption spectrum, the line shape may be fitted by a line shape expression.

A very important spectroscopic parameter is the *absorption coefficient* k , a measure of the absorbing power by an atom or a molecule. Remembering the previous relation we can write this quantity as:

$$k_{\nu,a} = S n_a \Phi(\nu - \nu_0) = S_n \Phi(\nu - \nu_0) \quad (2.9)$$

being n_a the number of molecules radiatively active per volume unit and S the strength of the line. S_n is a parameter that indicates the strength but for the total number of molecules per volume units and is measured in $m^{-1}s^{-1}$ units. Often can be more useful use the *mass absorption coefficient* defined as:

$$k_{\nu,a}^m = \frac{k_{\nu,a}}{\rho_a} = S \frac{n_a}{\rho_a} \Phi_i(\nu - \nu_0) = S^* \Phi_i(\nu - \nu_0) \quad (2.10)$$

where ρ_a is the absorber density and S^* is a new definition of line strength now expressed in $m^2 kg^{-1} s^{-1}$ units. While S is temperature dependent only, S_n e S^* are functions of concentration of the molecules.

So if we consider only LTE conditions, the molecular absorption can be written as:

$$k_{\nu,a} = \frac{S p \alpha_{L_0}}{\pi[(\nu - \nu_0)^2 + \alpha_{L_0}^2 p^2]} \quad (2.11)$$

In such an individual spectral line, the absorbing power approaches zero asymptotically at increasing distance in the line wings from the center. More generally, however, the absorbing power does not become zero between lines because of the overlapping effects of many lines.

2.2 Radiative energy transfer processes

The electromagnetic field can be regarded as an electromagnetic disturbance in the form of waves with a dual character: it exhibits an electric and a magnetic component. The components are in the form of oscillating fields, whose magnitude and direction is specified by the vector $\vec{E}$ and $\vec{H}$ respectively. In plane-polarized radiation these two vectors oscillate in mutually perpendicular directions. The electromagnetic field may also be considered as consisting of photons carrying energy.

In order to quantify the absorbed, transmitted or emitted radiation by a generic source we need to introduce some basilar relations between energy and radiative processes. This will be useful to understand the radiative transfer equation and all its properties described in next paragraphs.

2.2.1 The Irradiance

The *spectral irradiance* F_ν , measures the radiant energy flux transported through a given surface per unit area per unit time per unit wavelength.

Consider a surface dA with normal vector $\hat{n}$, if the surface is orthogonal to the generic $\hat{r}$ direction. All radiant energy traveling parallel to $\hat{r}$ crosses this surface and thus contributes to the irradiance with total efficiency. Energy traveling orthogonal and thus parallel to the surface, however, never crosses the surface and does not contribute to the irradiance at all. In general, the intensity F_ν projects onto the surface with an efficiency related to $\cos \theta = \vec{r} \cdot \hat{n}$.

The energy passing through the area can be written as:

$$F_\nu(\vec{r}, \hat{n}) = \frac{d^3 E}{dA dt d\nu} \quad \left[\frac{W}{m^2 Hz} \right] \quad (2.12)$$

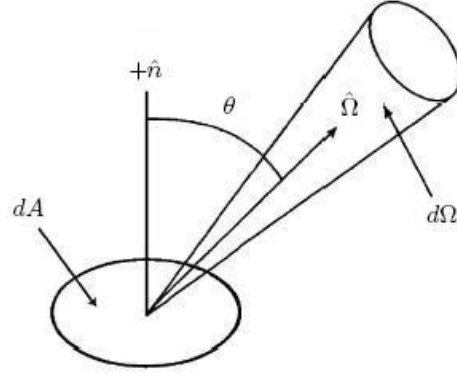


Figure 2.2: Example of radiation inside an infinitesimal solid angle $d\Omega$ along the direction $\hat{\Omega}$. The elemental area dA is also shown.

The irradiance per unit frequency F_ν over any given frequency range, $[\nu \text{ e } \nu + d\nu]$ is $F_\nu d\nu$ and the total irradiance is the integral over all the frequencies:

$$F(\vec{r}, \hat{n}) = \int_0^\infty F_\nu(\vec{r}, \hat{n}) d\nu \quad \left[\frac{W}{m^2} \right] \quad (2.13)$$

If we consider any given wavelength range $[\lambda \text{ e } \lambda + d\lambda]$, we can define the irradiance per unit wavelength F_λ , and the quantity $F_\lambda d\lambda$ the in the same way. In complete analogy, F_ν and $F_\nu d\nu$ if expressed in unit wavenumber.

The irradiance per unit frequency F_ν , is simply related to the other irradiance definitions. Being only different definition units they represent the same physical aspect of the energy, so we can write $F_\nu |d\nu| = F_\lambda |d\lambda| = F_{\tilde{\nu}} |d\tilde{\nu}|$ and the relations between these definitions:

$$F_\lambda(\vec{r}, \hat{n}) = F_\nu(\vec{r}, \hat{n}) \frac{d\nu}{d\lambda} = F_\nu(\vec{r}, \hat{n}) \frac{c}{\lambda^2} \quad \left[\frac{W}{m^2 \mu m} \right] \quad (2.14)$$

for the frequency-wavelength relation and:

$$F_{\tilde{\nu}}(\vec{r}, \hat{n}) = F_\nu(\vec{r}, \hat{n}) \frac{d\nu}{d\tilde{\nu}} = F_\nu(\vec{r}, \hat{n}) c \quad \left[\frac{W \text{ cm}}{m^2} \right] \quad (2.15)$$

for the frequency-wavenumber.

We remark that even if the expressions are different, they represent the same energy process.

2.2.2 The Radiance

The fundamental quantity defining the radiation field is the specific intensity of radiation L_ν .

Also known as *Radiance*, specific intensity measures the flux of radiant energy transported in a given direction per unit cross sectional area orthogonal to the beam per

unit time per unit solid angle per unit frequency⁴.

Consider light traveling in the direction through the point $\hat{\mathbf{r}}$. Construct an infinitesimal element of surface area dS intersecting $\hat{\mathbf{r}}$ and orthogonal to $\hat{\mathbf{\Omega}}$. The radiant energy dE crossing dS in time dt in the solid angle $d\Omega$ in the frequency range $[\nu \text{ e } \nu + d\nu]$ is related to L_ν by:

$$L_\nu(\vec{\mathbf{r}}, \hat{\mathbf{\Omega}}) = \frac{d^4 E(\Omega)}{dS \, dt \, d\nu \, d\Omega} \quad \left[\frac{W}{m^2 \, Hz \, sr} \right] \quad (2.16)$$

Very often however, it is not convenient to measure the radiant flux across surface orthogonal to $\hat{\mathbf{\Omega}}$, as in (2.16), when we consider properties of radiation fields with preferred directions. If instead, we measure the intensity orthogonal to an arbitrarily oriented surface element dA with surface normal $\hat{\mathbf{n}}$, then we must alter the expression of L_ν to account for projection of dS onto dA . If the angle between $\hat{\mathbf{n}}$ and $\hat{\mathbf{\Omega}}$ is θ then

$$\cos\theta = \vec{\mathbf{n}} \cdot \hat{\mathbf{\Omega}}$$

and the projection of dS onto dA yields

$$dA = dS \cos\theta$$

so that:

$$L_\nu(\vec{\mathbf{r}}, \hat{\mathbf{\Omega}}) = \frac{d^4 E(\Omega)}{dS \cos\theta \, dt \, d\nu \, d\Omega} \quad \left[\frac{W}{m^2 \, Hz \, sr} \right] \quad (2.17)$$

The Radiance is always a positive quantity.

When $\pi/2 < \theta < \pi$ ($\hat{\mathbf{n}} \cdot \hat{\mathbf{\Omega}} < 0$) in fact the energy flux (depending on Ω) is negative as well, so that the ratio remains positive.

The conceptual advantage is that the (2.17) builds in the geometric factor required to convert to any preferred coordinate system defined by dA and its normal $\hat{\mathbf{n}}$. In practice dA is often chosen to be the local horizon.

The radiation field is a seven-dimensional quantity, depending upon three coordinates in space, one in time, two in angle, and one in frequency. We can reduce the number of spatial dimensions from three to one by assuming a stratified atmosphere which is horizontally homogeneous and in which physical quantities may vary only in the vertical dimension, thus we replace $\hat{\mathbf{r}}$ by $\hat{\mathbf{z}}$.

This approximation is also known as a *plane-parallel* atmosphere, and comes with at least two important caveats: the first is the neglect of horizontal photon transport which can be important in inhomogeneous cloud and surface environments, the second is the neglect of path length effects at large solar zenith angles which can dramatically affect the mean intensity of the radiation field, and thus the atmospheric photochemistry.

With these assumptions, the intensity is a function only of vertical position and of direction, $L_\nu(\vec{\mathbf{r}}, \hat{\mathbf{\Omega}})$. The angular direction of the radiation is specified in terms of the polar angle θ and the azimuthal angle ϕ . The polar angle is the angle between $\hat{\mathbf{\Omega}}$ and the normal surface $\hat{\mathbf{n}}$ that defines the coordinate system.

The specific intensity of radiation traveling at polar angle and azimuthal angle in a

⁴Or even wavelength λ or wavenumber $\tilde{\nu}$ units

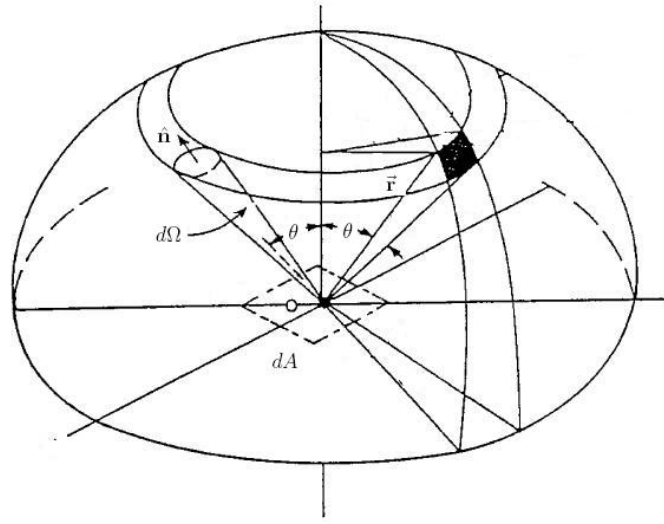


Figure 2.3: Geometry of the radiance from an emitting surface dA over all the hemisphere above. All the geometric parameters described in the text are shown.

plane parallel atmosphere is denoted by $L_\nu(\vec{r}, \hat{\Omega}, \theta, \phi)$ so the final expression of the specific intensity should be formally written as $L_\nu(\vec{r}, \hat{\Omega}, t, \nu, \theta, \phi)$.

Specific intensity is also referred to as *Intensity* only.

Further simplification of the intensity field is possible if it meets certain criteria. If L_ν is not a function of position $\hat{r}$ then the field is $L_\nu(\hat{\Omega}, t, \nu, \theta, \phi)$ and is said *homogeneous*, if it is not a function of direction $\hat{\Omega}$, then the expression is $L_\nu(\vec{r}, t, \nu, \theta, \phi)$ and the field is said *isotropic*.

Considering again an infinitesimal element of surface area dA and the energy fluxes crossing from an to it, the relations between Irradiance and Radiance can be written using the integration on all over two hemispheres above and below the surface. We can write:

$$d^3 E^\uparrow = \int_+ d^4 E(\Omega) \geq 0 \quad d^3 E^\downarrow = \int_- d^4 E(\Omega) \geq 0 \quad (2.18)$$

where the signs $+$ and $-$ mean the integral with versors normal to the surface defined by $+\hat{n}$ and $-\hat{n}$. Integrating on over the solid angle 4π and defining $\mu = \cos \theta$ we obtain:

$$F_\nu^\uparrow = \frac{d^3 E^\uparrow}{dA dt d\nu} = \int_0^{2\pi} \int_0^{\pi/2} L_\nu(\theta, \phi) \cos \theta d\Omega = \int_0^{2\pi} \int_0^1 L_\nu(\mu, \phi) \mu d\mu d\phi \quad (2.19)$$

$$F_\nu^\downarrow = \frac{d^3 E^\downarrow}{dA dt d\nu} = - \int_0^{2\pi} \int_{\pi/2}^\pi L_\nu(\theta, \phi) \cos \theta d\Omega = - \int_0^{2\pi} \int_{-1}^0 L_\nu(\mu, \phi) \mu d\mu d\phi \quad (2.20)$$

$$F_\nu = \int_0^{2\pi} \int_0^\pi L_\nu(\theta, \phi) \cos \theta d\Omega = \int_0^{2\pi} \int_{-1}^1 L_\nu(\mu, \phi) \mu d\mu d\phi \quad (2.21)$$

where the first expression is referred to the flux crossing the hemisphere above the surface, the second to the flux crossing the hemisphere below the surface and the third one is total spectral flux. The first two are always positive quantities.

If we consider the case of isotropic radiation, on all the point of the surface $L_\nu(\vec{r}, \hat{s}) = L_\nu = \text{cost}$ and we can rewrite the previous equations as:

$$F_\nu^\uparrow = L_\nu \int_0^{2\pi} \int_0^1 \mu d\mu d\phi = \pi L_\nu \quad (2.22)$$

$$F_\nu^\downarrow = -L_\nu \int_0^{2\pi} \int_{-1}^0 \mu d\mu d\phi = \pi L_\nu \quad (2.23)$$

$$F_\nu = L_\nu \int_0^{2\pi} \int_{-1}^1 \mu d\mu d\phi = 0 \quad (2.24)$$

In the isotropic case the total flux is zero.

Often it is convenient to consider a spectral radiance averaged on all the directions. In order to obtain this quantity is useful to define the energy spectral density. If dV and dA are an infinitesimal element of volume and area respectively and if the radiation travels a length $c dt$ (in dt), the infinitesimal energy in the time range $t, t+dt$ per frequency is:

$$dU_\nu = \frac{d^4 E}{dV d\nu} = \frac{L_\nu d\Omega}{c} \quad \left[\frac{J}{m^3 Hz} \right] \quad (2.25)$$

and the integral all over the solid angle is:

$$U_\nu(\vec{r}) = \int_{4\pi} dU_\nu = \int_{4\pi} \frac{L_\nu d\Omega}{c} = \frac{4\pi}{c} \bar{L}_\nu(\vec{r}) \quad \left[\frac{J}{m^3 Hz} \right] \quad (2.26)$$

where $\bar{L}_\nu(\vec{r})$ is the *average spectral radiance*, defined as:

$$\bar{L}_\nu = \frac{1}{4\pi} \int_{4\pi} L_\nu(\vec{r}, \theta, \phi) d\Omega \quad \left[\frac{W}{m^2 Hz} \right] \quad (2.27)$$

This quantity is proportional to the field energy density where the radiation is traveling.

2.2.3 Black Body radiation

It had long been observed that the surface of all bodies at a temperature greater than absolute zero (0 K) emits energy, in the form of thermal radiation.

These electromagnetic waves were thought to be due to the motion of electric charges near the surface of the radiating body. The study of radiation focused on the properties of a hypothetical *black body*, which is characterized by two main properties:

1. complete absorption of all incident radiation⁵.
2. maximum possible emission in all wavelengths in all directions.

⁵...hence the term black.

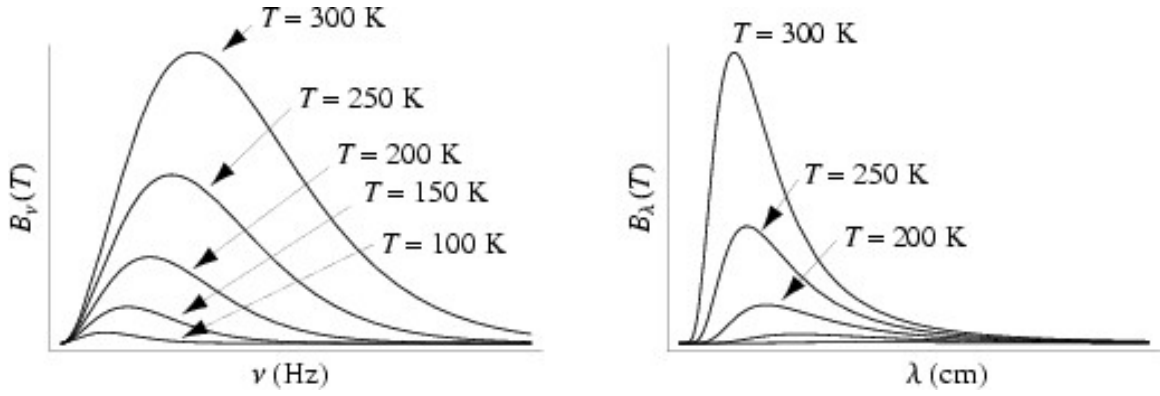


Figure 2.4: *Emission spectra for Black Bodies with relative temperatures. The difference in the Planck radiance curves when measured with respect to unit wavelength versus unit wavenumber is also shown.*

In other words, it is the perfect absorber and emitter of all radiation.

Many attempts, both empirical and theoretical in approach, were made in the years up to and about 1900 to understand the black body spectrum.

In 1879, Stefan had empirically found that the irradiance of a black body was related to the temperature of the body.

In 1884, Boltzmann produced a theoretical derivation of this relation.

Earliest accurate measurements of monochromatic irradiance are credited to Lummer and Pringsheim in 1899. They observed the now well-known emission spectra for black bodies at several different temperatures.

Anyway, there was a discrepancy between experiment data and theory.

The problem was resolved by Planck in 1901 assuming that electromagnetic harmonic oscillations can only exist in quanta and that oscillators emit energy only when changing from one to another of their quantized energy states.

Thus, in the course of his successful attempt at resolving certain discrepancies between the observed energy spectrum of thermal radiation and the predictions of the classical theory, Planck was led to the idea that a system executing simple harmonic oscillations only can have energies which are integral multiples of a certain finite amount of energy.

A closely related idea was later applied by Einstein in explaining the photo-electric effect (1905) and by Bohr in a theory which predicted with great accuracy many of the complex features of atomic spectra (1913).

The work of these three physicists, plus subsequent developments by de Broglie, Schroedinger and Heisenberg (1925), constitutes what is known as the quantum theory.

Quantum theory and the theory of relativity together comprise the two most significant features of modern physics.

From a mathematical point of view, the *Planck's law* can be written as:

$$B_\nu(T) = \frac{2h\nu^3}{c^2(e^{h\nu/k_B T} - 1)} \quad \left[\frac{W}{m^2 \text{ Hz sr}} \right] \quad (2.28)$$

in wavenumber units or

$$B_\lambda(T) = \frac{2hc^2}{\lambda^5(e^{hc/k_B\lambda T} - 1)} \left[\frac{W}{m^2 \mu m sr} \right] \quad (2.29)$$

in wavelength units.

The Planck function, describes the intensity of blackbody radiation as a function of temperature and frequency. In the expression of the radiance $B(T)$, h is the Planck's constant⁶, c is the speed of light⁷, k_B is the Boltzmann's constant⁸ e T is the body temperature in Kelvin units.

From this very important formulation many other relation have been derived.

The Planck function in fact, has interesting behavior in both the high and the low energy photon limits.

Wien's displacement law

The peak of Planck function curve shifts to shorter wavelengths with an increase in temperature. The wavelength max for which the Planck function peaks at a given temperature T can be found from Planck's law by differentiating it with respect to λ and equating the result to zero:

$$\frac{\partial B_\lambda}{\partial \lambda} = 0 \quad (2.30)$$

this yields the nonlinear equation $x = 5(1 - \exp(-x))$ where $x = hc/k_B(\lambda_{max} T)$ whose solution is $x = 4.9651$. Therefore:

$$\lambda_{max} T = 2897.8 \quad [\mu m K] \quad (2.31)$$

which is the *Wien's displacement law*. This law indicates that the wavelength of maximum Planck radiance varies inversely with temperature.

The Planck radiance at the Wien wavelength λ_{max} varies as temperature to the fifth power:

$$B_{\lambda_{max}} = \frac{a}{\pi} T^5 = 4.096 T^5 \left[\frac{W}{m^2 \mu m sr} \right] \quad (2.32)$$

where $a = 12.87 W/(m^2 sr K^5 \mu m)$.

The radiative temperature of the surface of the sun is roughly 5780 K . Applying Wien's Law at the Sun's surface temperature, one finds the maximum Planck radiance to be at 0.5 μm which is near the center of the visible region of the spectrum. Since the sun radiates nearly as a black body, we can say that the solar energy reaching the earth is a maximum in the visible region.

Wien's displacement law derives its name from the fact that as the temperature increases, the point of maximum intensity of the black body curve is displaced toward the shorter wavelengths.

Since the wavelength of the maximum value determines the color perceived while observing the complete spectrum, we have an explanation for the transition in color

⁶ $h = 6.626 \times 10^{-34} Js$.

⁷ $2.99792 \times 10^8 ms^{-1}$.

⁸ $1.38054 \times 10^{-23} JK^{-1}$.

of a heated iron bar from red to a white glow with increased heat.

As the temperature is raised the longer wavelength red light becomes visible first. Then higher temperatures make additional wavelengths visible.

Finally, when the temperature is sufficiently high, the radiation consists of a mixture of all the visible wavelengths and, hence, appears white hot.

For similar reasons, the filament of an incandescent lamp must be heated to thousands of degrees K in order to be an efficient emitter of visible light, while infrared lamps operate at lower temperatures.

Stefan-Boltzmann law

The black body irradiance is obtained by integrating the Planck function over all wavelengths:

$$F_{bb} = \pi \int_0^\infty B_\nu d\nu \quad (2.33)$$

if we use the expression 2.32 instead of B_ν we obtain:

$$F_{bb} = \sigma_B T^4 \quad (2.34)$$

with $\sigma_B = 5.6703 \times 10^{-8} W m^{-2} K^{-4}$ is the Stefan-Boltzmann constant. We here mention other two special cases of the Wien's formulation.

In the near infrared region and beyond into the visible and ultraviolet regions the exponent in the Planck function is large and hence $h\nu \gg k_B T$, this yields the *Wien's Radiation Law*:

$$B_\nu = \frac{2h\nu^3}{c^2 e^{h\nu/k_B T}} \left[\frac{W}{m^2 Hz sr} \right] \quad (2.35)$$

very useful when $\lambda \leq 10 \mu m$, or in general when $\lambda T \leq 0.5 cm K$.

In the microwave region of the electromagnetic spectrum, the exponent in the Planck function is small, and hence one can make the approximation $h\nu \ll k_B T$ and this yields the *Rayleigh-Jeans Radiation Law*:

$$B_\lambda = \frac{2 c k_B T}{\lambda^4} \left[\frac{W}{m^2 \mu m sr} \right] \quad (2.36)$$

Note that in the Rayleigh-Jeans region the Planck function is linear to T .

Brightness temperature

Every time an instrument measures a radiance coming from a direction $\hat{s} = \hat{s}(\theta, \phi)$ is then possible define the quantity:

$$T_B(\theta, \phi) = L_\nu \frac{\lambda^2}{2 k_B} \quad (2.37)$$

This because often it can be very useful to know the temperature that corresponds to a particular B_λ value. This temperature is determined by inverting the Planck's function:

$$T_B = \frac{hc}{k_B \lambda \log[(hc^2/\lambda^5 B_\lambda) + 1]} \quad (2.38)$$

The temperature derived is called *brightness temperature* because of its historical connection with radio astronomy; however, the terms radiance temperature or equivalent black body temperature are also frequently used.

As we have seen from Planck's Law, as temperature increases the radiance also increases and the percentage increase varies as a function of wavelength and temperature.

2.3 Radiative processes

Much of what has been presented so far has assumed a knowledge of metrics of the radiative properties of entire systems.

These metrics describe normalized properties of a system and thus are somewhat more fundamental than absolute quantities (like transmitted irradiance) which may, for example, change depending on some other quantities related to the systems.

We can consider four distinct processes to characterize the radiative energy budget for a real body. These four quantities are:

1. **Emission**
2. **Absorption**
3. **Reflection**
4. **Transmission**

We shall define these quantities first, and then integrate these definitions with the appropriate weighting to obtain the final expressions.

2.3.1 Emission

As we noted earlier, blackbody radiation represents the upper limit to the amount of radiation that a real substance may emit at a given temperature T_{Surf} .

If $L_\nu^e(\hat{\Omega}) dA \cos \theta d\Omega$ is the power emitted by an infinitesimal surface dA inside the solid angle $d\Omega$ along the direction $\hat{\Omega}$, the power for a black body surface will be $B_\nu(T_{Surf}) dA \cos \theta d\Omega$.

At any given wavelength, *emissivity* is defined as the ratio of the actual emitted radiance, $L_\nu^e(\hat{\Omega})$ to that from an ideal blackbody $B_\nu(T_{Surf})$:

$$\epsilon_\nu(\hat{\Omega}, T_{Surf}) = \frac{L_\nu^e(\hat{\Omega}) dA \cos \theta d\Omega}{B_\nu(T_{Surf}) dA \cos \theta d\Omega} = \frac{L_\nu^e(\hat{\Omega})}{B_\nu(T_{Surf})} \quad (2.39)$$

depending by the direction of the emission, by surface temperature T_{Surf} , by frequency ν and other quantities as refractive index.

In case of *Rayleigh-Jeans* approximation, (2.39) become:

$$\epsilon_\nu(\hat{\Omega}, T_{Surf}) = \frac{T_{Surf}(\hat{\Omega})}{T_{Surf}^{bb}} \quad (2.40)$$

A surface with $\epsilon_\nu(\hat{\Omega}, T_{Surf}) = 1$ for any frequency and all the angles is a black body, if $\epsilon = \text{cost} < 1$, independent by frequency, it is a *grey body*.

We mention the *spectral flux emissivity* defined as the ratio between the flux emitted by a real body and the flux emitted by a black body at the same temperature T_{Surf} integrated all over the hemisphere (positive or negative):

$$\epsilon_\nu(2\pi, T_{Surf}) = \frac{1}{\pi} \int_+ \epsilon_\nu(\hat{\Omega}, T_{Surf}) \cos \theta d\Omega \quad (2.41)$$

It is clear that $\epsilon_\nu(2\pi, T_{Surf})$ is a surface property. In the infrared part of the electromagnetic spectrum almost all the surface are good emitters.

2.3.2 Absorption

If we consider the light incident inside a solid angle $d\Omega_o$ along the direction $\hat{\Omega}_o$, the power that will be absorbed is $L_\nu^a(\hat{\Omega}_o) dA \cos \theta_o d\Omega_o$.

We define the *absorbance* as the ratio between the absorbed power and the incident one:

$$\alpha_\nu(\hat{\Omega}_o, T_{Surf}) = \frac{L_\nu^a(\hat{\Omega}_o) dA \cos \theta_o d\Omega_o}{L_\nu(\hat{\Omega}_o) dA \cos \theta_o d\Omega_o} = \frac{L_\nu^a(\hat{\Omega}_o)}{L_\nu(\hat{\Omega}_o)} \quad (2.42)$$

and the *spectral flux absorbance* as:

$$\alpha_\nu(2\pi, T_{Surf}) = \frac{\int_- \alpha_\nu(\hat{\Omega}_o, T_{Surf})_\nu(\hat{\Omega}_o) \cos \theta_o d\Omega_o}{F_\nu} \quad (2.43)$$

If the incident radiation is of a *black body* at T_{Surf} or in general is isotropic, than the previous relation become:

$$\alpha_\nu(2\pi, T_{Surf}) = \frac{1}{\pi} \int_- \alpha_\nu(\hat{\Omega}_o, T_{Surf}) \cos \theta_o d\Omega_o \quad (2.44)$$

similar to the (2.41).

If the source of radiation is in thermal equilibrium with the absorbing medium, then:

$$\alpha_\nu(\hat{\Omega}, T_{Surf}) = \epsilon_\nu(\hat{\Omega}, T_{Surf}) \quad (2.45)$$

This is often referred to as *Kirchhoff's Law* that, in qualitative terms, it states that materials which are strong absorbers at a given wavelength are also strong emitters at that wavelength. Similarly weak absorbers are weak emitters.

2.3.3 Reflection

This third process can be quantified by the *Bidirectional Reflectance Distribution Function* (BRDF).

This represents the ratio between the reflected intensity along the direction $\hat{\Omega}$ and the energy of the beam incident along $\hat{\Omega}_o$ on the surface:

$$\rho_\nu(\hat{\Omega}_o, \hat{\Omega}) = \frac{dL_\nu^r(\hat{\Omega})}{L_\nu(\hat{\Omega}_o) \cos \theta_o d\Omega_o} \quad (2.46)$$

as such, ρ_ν is a function of frequency, incident angle, and scattered angle. $dL_\nu^r(\hat{\Omega})$ represents only an infinitesimal fraction of $L_\nu(\hat{\Omega})$ generated by the incident radiation along the direction $\hat{\Omega}$.

From (2.46) it is clear that the total reflected intensity in any particular direction $\hat{\Omega}$ is the sum of contributions from all incident beams on the surface from directions $\hat{\Omega}_o$ that have a finite probability of reflecting into $\hat{\Omega}$:

$$L_\nu^r(\hat{\Omega}) = \int_+ dL_\nu^r(\hat{\Omega}) = \int_+ \rho_\nu(\hat{\Omega}_o, \hat{\Omega}) L_\nu(\hat{\Omega}_o) \cos \theta_o d\Omega_o \quad (2.47)$$

where the integration is on all over the hemisphere. The dependence on two directions and on frequency makes it a difficult property to measure. Fortunately many surfaces found in nature obey simpler reflectance properties.

A *Lambertian surface* is one whose reflectance is independent of both incident and reflected directions. The reflectance of a *Lambertian surface* depends only on frequency:

$$\rho_\nu(\hat{\Omega}_o, \hat{\Omega}) = \rho_{L,\nu} \quad (2.48)$$

this means that the intensity of the reflection is:

$$L_\nu^r(\hat{\Omega}) = \rho_{L,\nu} \int_+ L_\nu(\hat{\Omega}_o) \cos \theta_o d\Omega_o = \rho_{L,\nu} F_\nu \quad (2.49)$$

As expected, the intensity reflected from a Lambertian surface depends only on the incident irradiance, and not at all on the details of the angular distribution of the incident intensity field.

A *Fresnel surface* is one whose reflectance occurs only when $\theta_o = \theta$ with θ_o and θ incident and reflected angle, respectively. The *Fresnel reflectance* can be written as:

$$\rho_\nu(\hat{\Omega}_o, \hat{\Omega}) = \frac{\rho_{F,\nu}(\theta)}{\cos \theta} \quad (2.50)$$

so that:

$$L_\nu^r(\hat{\Omega}) = \int_+ L_\nu(\hat{\Omega}_o) \frac{\rho_{F,\nu}(\theta)}{\cos \theta} \quad (2.51)$$

In general, a surface will have a specular component and a reflected one so that the general expression for the reflectance can be expressed by:

$$\rho_\nu(\hat{\Omega}_o, \hat{\Omega}) = \rho_{L,\nu} + \frac{\rho_{F,\nu}(\theta)}{\cos \theta} \quad (2.52)$$

a diffuse component $\rho_{L,\nu}$ and a specular one $\rho_{F,\nu}(\theta)$.

The reflectance of a surface illuminated by a collimated source such as the Sun is of great interest in planetary studies and in remote sensing. For an incident collimated beam along the direction $\hat{\Omega}_o$, the diffusely reflected flux intensity can be expressed by $F_\nu = F_\nu^o \cos \theta_o$. The final intensity will be:

$$L_\nu^r(\hat{\Omega}) = F_\nu^o \cos \theta_o \rho_\nu(\hat{\Omega}_o, \hat{\Omega}) \quad (2.53)$$

and the total flux:

$$F_\nu^r = \int_+ L_\nu^r(\hat{\Omega}) \cos \theta d\Omega = F_\nu^o \cos \theta_o \int_+ \rho_\nu(\hat{\Omega}_o, \hat{\Omega}) \cos \theta d\Omega \quad (2.54)$$

that permits to define the *albedo* or *flux reflectance* as:

$$\rho_\nu(\hat{\Omega}_o, 2\pi) = \frac{F_\nu^r}{F_\nu^o \cos \theta_o} = \int_+ \rho_\nu(\hat{\Omega}_o, \hat{\Omega}) \cos \theta \, d\Omega \quad (2.55)$$

This quantity is often called *plane albedo*. This because when the reflecting body is of finite size then the corresponding ratio of reflected to incident fluxes is more complicated because it contains “edge effects” as diminishing contributions from planetary limbs. In this case other quantity result more appropriate as the *spherical albedo*, *planetary albedo* or *bond albedo*, to describe the behavior of an entire planetary disk illuminated by collimated sunlight. In general, a surface will have an absorption component and a reflected one so that the expression of the fluxes can be expressed as:

$$F_\nu^a = \int_+ L_\nu(\hat{\Omega}_o) \alpha_\nu(\hat{\Omega}_o, T_{Surf}) \cos \theta_o \, d\Omega_o \quad (2.56)$$

$$F_\nu^r = \int_+ L_\nu(\hat{\Omega}_o) \rho_\nu(\hat{\Omega}_o, \hat{\Omega}) \cos \theta_o \, d\Omega_o \quad (2.57)$$

so that for the total flux:

$$F_\nu = F_\nu^a + F_\nu^r \quad (2.58)$$

now, remembering that $F_\nu = \int_+ L_\nu(\hat{\Omega}_o) \cos \theta_o \, d\Omega_o$, we obtain:

$$\alpha_\nu(\hat{\Omega}_o, T_{Surf}) + \rho_\nu(\hat{\Omega}_o, 2\pi) = 1 \quad (2.59)$$

this is the relation between the reflectance and the directional absorbance. We even mention the flux emitted by a surface:

$$F_\nu^e = \int_+ B_\nu(T_{Surf}) \epsilon_\nu(\hat{\Omega}, T_{Surf}) \cos \theta \, d\Omega \quad (2.60)$$

where $B_\nu(T_{Surf})$ is the well known black body intensity, depending by surface temperature only.

2.3.4 Transmission

Again as for reflection, if we consider a beam along $\hat{\Omega}_o$ with energy $L_\nu(\hat{\Omega}_o) \cos \theta_o \, d\Omega_o$ and $dL_\nu^t(\hat{\Omega})$ is the fraction of energy transmitted along the direction $-\hat{\Omega}$, we define *transmittance*:

$$\mathcal{T}_\nu(\hat{\Omega}_o, \hat{\Omega}) = \frac{dL_\nu^t(\hat{\Omega})}{L_\nu(\hat{\Omega}_o) \cos \theta_o \, d\Omega_o} \quad (2.61)$$

if we know $\mathcal{T}_\nu(\hat{\Omega}_o, \hat{\Omega})$, we can obtain the intensity along $-\hat{\Omega}$ as:

$$L_\nu^t(\hat{\Omega}) = \int_- dL_\nu^t(\hat{\Omega}) = \int_- \mathcal{T}_\nu(\hat{\Omega}_o, \hat{\Omega}) L_\nu(\hat{\Omega}_o) \cos \theta_o \, d\Omega_o \quad (2.62)$$

Just like the reflectance, we can split this quantity in a direct component and a diffuse one. Considering again the (2.59) we have:

$$\alpha_\nu(\hat{\Omega}_o, T_{Surf}) + \rho_\nu(\hat{\Omega}_o, 2\pi) + \mathcal{T}_\nu(\hat{\Omega}_o, 2\pi) = 1 \quad (2.63)$$

due to conservation of energy.

2.4 Radiative Transfer Equation

In general, Radiative transfer serves as a mechanism for exchanging energy between the atmosphere and the underlying surface and between different layers of the atmosphere.

Infrared radiation emitted by the atmosphere and intercepted by satellite sensors is the basis for remote sensing of the atmospheric temperature structure. The radiance leaving the planet-atmosphere system which can be sensed by a satellite borne radiometer is the sum of radiation emissions from the surface (if any...) and each atmospheric level that are transmitted to the top of the atmosphere.

Radiative transfer theory has been recognized as the principal modeling method that accounts for the solar radiation in the atmosphere.

In order to understand the relations between the quantities described in the previous paragraph and how is possible obtain physical informations about the atmospheric parameters from the observation is useful give some notions about the Radiative Transfer Equation and its expressions. If we consider again the quantity $L_\nu(\vec{r}, \hat{s})$, incident on an infinitesimal volume of length ds , we can recognize four main processes involved in it:

- process A : absorption of the incident radiation.
- process B : scattering of the incident radiation outside the volume.
- process C : scattering of the incident radiation inside the volume.
- process D : Plank's emission due to the matter temperature T .

the total process can be written as:

$$\frac{dL_\nu}{ds} = A + B + C + D \quad (2.64)$$

where A and B are negative (energy is lost) while C and D are positive. All the quantities depend on frequency ν .

2.4.1 Extinction

A is the process where absorption occurs.

Remembering the coefficient expressed in the (2.11), we can define other two important parameters: the *optical path*, defined as the integral of the absorption coefficient along the radiation optical path between the point s_1 and s_2 :

$$\tau_{\nu,a}(s_1, s_2) = \int_{s_1}^{s_2} k_{\nu,a} ds \quad (2.65)$$

The optical path measures the amount of extinction a beam of light experiences traveling between two points. When $\tau_\nu < 1$ the path is said to be optically thick. The most frequently used form of optical path is the *optical depth*. The optical depth is the vertical component of the optical path and measures extinction between vertical levels.

For historical reasons, the optical depth in planetary atmospheres is defined $\tau_\nu = 0$ at the top of the atmosphere. This convention reflects the astrophysical origin of much of radiative transfer theory.

Much like pressure, τ_ν is a positive definite coordinate which increases monotonically from zero at the top of the atmosphere to its surface value.

The second parameter is the *monochromatic transmittance* defined as:

$$\mathcal{T}_{\nu,a}(s_1, s_2) = e^{-\int_{s_1}^{s_2} k_{\nu,a} ds} = e^{-\tau_{\nu,a}(s_1, s_2)} \quad (2.66)$$

sometimes, the absorbing gaseous species in the atmosphere are expressed by the *optic mass* along the vertical path:

$$u_a(z_1, z_2) = \int_{z_1}^{z_2} \rho_a dz = \frac{1}{g} \int_{p_1}^{p_2} w_a dp \quad (2.67)$$

where z_1 and z_2 are the altitude of the point p_1 and p_2 , g is the gravity value and $w_a = \rho_a/\rho$ is the *mixing ratio* that indicates the percentage of a specie with the total atmosphere.

The optical depth depend on the scattering as well and a more general definition as a function of the altitude z is:

$$\tau_\nu(z_1, z_2) = \int_{z_1}^{z_2} k_{\nu,ext}(z) dz = \int_{z_1}^{z_2} k_{\nu,ext}^m(z) \rho_a(z) dz = \int_{z_1}^{z_2} \sigma_{\nu,ext}(z) n_a(z) dz \quad (2.68)$$

where n_a is the number of molecules per volume unit of the absorbing specie and $\sigma_{\nu,ext}$ is defined as the *extinction cross section* per single particle.

By convention, τ_ν is positive definite but it may be positive or negative. If this seems confusing, consider the analogy with atmospheric pressure: pressure increases monotonically from zero at the top of the atmosphere, and we often express physical concepts such as the temperature lapse rate in terms of negative pressure gradients.

2.4.2 Beer-Lambert Law

In the absence of scattering, the absorption of parallel beam radiation of intensity dL_ν as it passes downward through a horizontal layer of gas of infinitesimal thickness ds is proportional to the number of molecules per unit area that are absorbing radiation along the path.

This relation can be expressed in the form:

$$dL_\nu^{abs} \propto -L_\nu ds \quad (2.69)$$

representing the extinction law in differentiating form.

The term *extinction coefficient* k_{ext} indicates the proportional constant of the (2.69). The coefficient k_{ext} is a measure of the fraction of the gas molecules per unit wavelength interval that are absorbing radiation at the wavelength in question. It is a measure of the cumulative depletion that the beam of radiation has experienced as a result of its passage through the layer and it is a function of composition, temperature, and pressure of the gas within the layer.

We now define the *Beer-Lambert law* as:

$$\frac{dL_\nu}{ds} = -k_\nu^{ext} L_\nu = -(k_\nu^{abs} + k_\nu^{sct}) L_\nu \quad (2.70)$$

where the coefficient takes into account the absorption and the scattering as well. The previous expression represents the A and B processes of the (2.64). Moreover, we define the *mass extinction coefficient* k_{ext}^m defined by:

$$k_{ext}^m = \frac{k_{ext}}{\rho_a} \quad [m^2 Kg^{-1}] \quad (2.71)$$

we note that the cross section σ_{ext} defined in the (2.68) is related to the extinction coefficient by:

$$\sigma_{ext} = \frac{k_{ext}}{n_a} \quad [m^2] \quad (2.72)$$

We can now integrate the (2.70) for a vertical path:

$$L_\nu(s, \hat{\Omega}) = L_\nu(0, \hat{\Omega}) e^{-\tau_s} \quad (2.73)$$

so that

$$\mathcal{T}_s = e^{-\tau_s} \quad (2.74)$$

This relation states that radiance decreases monotonically with increasing path length through the layer from 0 to s .

$\mathcal{T}_s$, is the *Transmittance*, the ratio between the intensity at two different altitudes.

2.4.3 Source function

A and B represent processes where the energy is lost and their contributions are negative in the total energy balance.

If we consider the emission processes C and D inside the infinitesimal volume in analogy with the (2.69) we have:

$$dL_\nu^{ems} \propto ds \quad (2.75)$$

where the proportional constant in this case is given by the **emission coefficient** $j_\nu(\vec{r}, \hat{\Omega}) [W m^{-3} Hz^{-1} str^{-1}]$.

This is the emerging energy from an infinitesimal volume of length ds and area dA at time dt inside the solid angle $d\Omega$ along the direction $\hat{\Omega}$.

From this quantity we can define the *Source function* as:

$$S_\nu = \frac{j_\nu(\vec{r}, \hat{\Omega})}{k_\nu^{ext}} \quad (2.76)$$

so that we can write:

$$\frac{dL_\nu}{ds} = -k_\nu^{ext} L_\nu + k_\nu^{ext} S_\nu \quad (2.77)$$

or in equivalent optical depth form as:

$$\frac{dL_\nu}{d\tau} = -L_\nu + S_\nu \quad (2.78)$$

We distinguish between the S_ν due to scattering and thermal emission.

2.4.4 Scattering

The C process is due to scattering.

The direction of the photon after the interaction with the matter is usually not the same as the incoming direction. Scattering is the contribution of the radiance coming from all the directions $\hat{\Omega}'$ that is diffused along the direction $\hat{\Omega}$.

Being the radiance incident on the area dA along $\hat{\Omega}'$ at time dt in the frequency range $d\nu$:

$$d^4 E' = L_\nu(\hat{\Omega}') dA dt d\nu d\Omega'$$

for the part of energy diffused in all the directions we can write:

$$k_{sct} ds d^4 E'$$

if we define γ_{sct} as the *scattering angle*, the angle between the incident radiation defined by (θ, ϕ) and the outgoing one defined by (θ', ϕ') and with $P(\gamma_{sct})$ the *Phase function*⁹, a quantity describing the angular dependence by (θ', ϕ') , we can define the *scattering emission coefficient* as:

$$j_\nu^{sct} = k_{sct} \int_{4\pi} P(\hat{\Omega}, \hat{\Omega}') L_\nu(\hat{\Omega}) d\Omega \quad (2.79)$$

and the quantity:

$$S_\nu^{sct} = \frac{j_\nu^{sct}}{k_\nu^{ext}} = \frac{k_\nu^{sct}}{k_\nu^{ext}} \int_{4\pi} P(\hat{\Omega}, \hat{\Omega}') L_\nu(\hat{\Omega}) d\Omega \quad (2.80)$$

as *scattering source function*.

In the end the process C can be expressed as:

$$\frac{dL_\nu}{ds} = k_\nu^{sct} \int_0^{2\pi} \int_0^\pi L_\nu(\theta, \phi) P(\gamma_{sct}) \sin \theta d\theta d\phi = k_\nu^{sct} L_\nu^{dif} \quad (2.81)$$

where L_ν^{dif} is the average radiance weighted by the Phase function.

2.4.5 Thermal emission

For a body in local thermodynamic equilibrium the amount of thermal energy emitted must be equal to the energy absorbed; otherwise the body would heat up or cool down in time, contrary to the assumption of equilibrium.

⁹Because we assume that after the interaction between the radiation and the scattering particle the outgoing radiation is deflected along any direction, this function need to be normalized over the entire solid angle 4π through an integration over Ω :

$$\frac{1}{4\pi} \int_{\Omega} P(\gamma_{sct}) d\Omega = 1.$$

Be careful, many books normalize it directly to 1:

$$\int_{\Omega} P(\gamma_{sct}) d\Omega = 1.$$

At temperature T the radiance will be $L_\nu^{bb} = B_\nu(T)$ and the because equilibrium radiation will be uniform and isotrope so that $dL_\nu/ds = 0$ but from the (2.78) this means that:

$$\frac{dL_\nu}{d\tau_{ems}} = 0 = -L_\nu + S_\nu \quad L_\nu = S_\nu$$

but

$$L_\nu = B_\nu(T)$$

and

$$B_\nu(T) = S_\nu \quad (2.82)$$

this means that not only $B_\nu(T)$ describes the radiation field but it is the source function as well.

if we consider the term of only emission S_ν^{ems} due to the radiance of the medium it will depende from the temperature only. Remembering the *Kirchhoff's Law* the coefficient j_ν^{ems} will be proportional to the Planck function:

$$j_\nu^{ems} = k_\nu^{abs} B_\nu(T) \quad (2.83)$$

being k_ν^{abs} the absorption coefficient. For the variation of radiance due to the emission we can write:

$$\frac{dL_\nu}{ds} = k_\nu^{abs} B_\nu(T)$$

So the thermal part of the source function become:

$$S_\nu^{ems} = \frac{j_\nu^{ems}}{k_\nu^{sct}} = \frac{k_\nu^{abs}}{k_\nu^{ext}} B_\nu(T) \quad (2.84)$$

representing the last contribution D of the final expression.

2.4.6 Final expression

We can now consider again the (2.64) in an explicit form.

Before that, some very important parameters, linear combination of the previous ones, need to be defined. These parameters are:

$$\tilde{\alpha}_\nu = k_\nu^{abs} / k_\nu^{ext} \quad (2.85)$$

$$\tilde{\omega}_\nu = k_\nu^{sct} / k_\nu^{ext} \quad (2.86)$$

bounded by the relation $\tilde{\alpha}_\nu = 1 - \tilde{\omega}_\nu$ and where $\tilde{\alpha}_\nu$ is the *absorption quantity* and $\tilde{\omega}_\nu$ the *single scattering albedo*.

With these new definitions for the final expression of the radiative transfer equation we can write the (2.64) in optical depth terms as:

$$\frac{dL_\nu}{d\tau} = -L_\nu(\theta, \phi) + \tilde{\alpha}_\nu B_\nu(T) + \tilde{\omega}_\nu \int_0^{2\pi} \int_0^1 L_\nu(\mu', \phi') P(\gamma_{sct}) d\mu' d\phi' \quad (2.87)$$

valid for a vertical path and for a scattering geometry defined by μ' e ϕ' being $\mu' = \cos \theta'$.

This is the differential form of the radiative transfer equation in a plane parallel atmosphere and is valid for all angles. From the integration of the (2.87), the final expression of radiance arises mainly from the knowledge of the Planck function and the spectral transmittance.

The Planck function consists of temperature information, while the transmittance is associated with the absorption coefficient and density profile of the relevant absorbing gases.

Obviously, the observed radiance contains the temperature and gaseous profiles of the atmosphere, and therefore, the information content of the observed radiance from satellites must be physically related to the temperature field and absorbing gaseous concentration. There is no unique solution for the detailed vertical profile of temperature or an absorbing constituent for many reasons.

First, because the outgoing radiances arise from relatively deep layers of the atmosphere, then the radiances observed within various spectral channels come from overlapping layers of the atmosphere and are not vertically independent of each other and, more, measurements of outgoing radiance possess errors.

As a consequence, there are a large number of analytical approaches to the profile retrieval problem. The approaches differ both in the procedure for solving the set of spectrally independent radiative transfer equations and in the type of ancillary data used to constrain the solution to insure a good result.

However, the explication of the mathematical formalism of the Radiative Transfer Equation is out of the competence of this thesis.

The Model

In principle, all the measured data (earth based, airborne, from space, spacecraft based or whatever) would be completely useless without any good theoretical model to convalidate them.

The opposite is true as well.

A model can be said a good model if it is justified by observations.

New scientific knowledges occur only when those two distinct aspect are in agreement each other, becoming the same thing.

In this chapter a Radiative Transfer Model (RTM) for the atmosphere of Saturn is presented.

Even if we have tested it with the Saturn data only, one of the effort of our work has been the generality of the model and the complete adaptability to the other Giant Planets data as well.

From the procedures to obtain the outputs to the informatic architecture of our procedures, everything has been modeled for a total interchangeability.

The VIMS spectro-images data of the Cassini-Huygens mission to the ringed planet are used for comparison and RTM validation.

The model with all the methodologies used for our purpose and how the simulated spectra are created will be illustrate in the next paragraphs. Synthetic spectra are the base and the final output of all our work, they are the fundamental part for the comparison with the data produced by the instrument.

It will be also shown how the forward model solves the radiative transfer equation (in an adapted form for our goals) and all the practical choices made to get the final state of the model itself.

3.1 Purpose of the work

Spectroscopic remote sensing is one of the most powerful techniques to get physical information of a distance target. Observing the radiation emerging from a planet, a variety of physical quantities can be retrieved.

Once the measured data are available however, we need to produce a model which properly simulate what the instrument measures in order to retrieve specific parameters and to get information on the atmosphere in general.

The aim of this work is the construction and validation of a Radiative Transfer model for the Giant Planets atmosphere using the data of the spectrometer VIMS described before.

Taking a look at the Saturn's images produced by VIMS the huge variety of atmospheric condition is evident. Spectra of different intensity and shape show different physical phenomena occurring on the planet.

The model we present here is made with the aid of some simplifying assumptions and validity conditions. Many physical processes occur in real data that cannot be reproduced easily by our model.

As said before all the work can be separate in two distinct parts:

- Construction of the model itself.
- Validation of the model with the instrument data.

The first task is the object of this chapter.

Our final goal is to simulate the radiance spectra a specific instrument would measure at the same conditions imposed *a priori*.

The observed spectrum of a planet is the result of the contribution of many different processes that have to be take into account in the model. In order to better understand the choices we have made and that will be explained in detail next pages, we can summarize all the construction of the model in different steps:

- Atmospheric composition: main molecules and isotopes involved and definition of the *continuum* level. Abundances and profiles.
- Thermal structure: pressure profile as a function of temperature.
- Spectroscopic molecular parameters and their correction to the Giant Planets atmospheric conditions.
- Definition of the spectral range (VIMS instrument bandwidth) and its spectral resolution.
- Calculation of the radiative quantities for the single gaseous species and the total atmosphere. Definition of sounded levels as a function of wavelengths.
- Implementation of all the boundary conditions imposed and the simplifying assumptions.
- Aerosols content and profiles. Nature of the aerosols and effects of the clouds opacity to the simulated spectra.
- Computation of the atmospheric outgoing radiance solving the Radiative Transfer equation under different options and taking into account all the results coming from the previous steps.
- Convolution of the high resolution spectra with the instrumental function for the final comparison.

Once the convoluted synthetic spectra have been available, a spectral databank has been created in order to find the best fit between the chosen observations spectra and the elements of the database.

3.2 The ARS software

The code we use for our purpose is ARS, acronym of Atmosphere Radiation Spectrum. Basically, it is a set of routines written in fortran 77 and C able to perform computations of several physical quantities and to solve the radiative transfer equation under different conditions.

Using different packages separately, the code can compute the opacity of gaseous species and aerosols, the transmittance and the radiance spectra with only LTE ¹ conditions. The code was originally created and developed by N.I. Ignatiev (IKI RAN-Moscow) to study the data of the PFS interferometer, instrument of the Mars Express mission's payload, is now used for other planetary atmospheres by many research teams.

In general the radiative transfer problem can be subdivided in two distinct and independent tasks:

- Computation of physical properties.
- Solution of the radiative transfer equation itself.

From a informatic point of view, ARS uses many packages and modules. Every package requires a set of initialization files (*.ini) and as sequential boxes, the output of the previous box is the input of the subsequent one.

Anyway, being the detailed description of the code out of the purpose of this work, the main packages and a little explanation of them can be summarized as follow:

Arshls : This package extracts spectral lines data from a spectroscopic database and converts them into a reduced format file. It is able to change isotopic ratios and Lorentz line half widths. Moreover it can discard all the lines with intensity lower than a chosen value. Another important options is the line wings cutoff, in order to consider the main contribution of the information only. It can work with different databases also.

Arsv : Once the lines are extracted, next important step is the creation of a grid with different resolutions. Arsv can create uniform or combined wavenumber grid, according to different line parameter (positions, widths, strengths, line shape, etc...) in wavenumber units only. It is possible to have uniform spectral range or combine ranges of different resolution. Because the very different number of lines in different parts of a selected spectral range, this last option can be very useful in order to save computational time.

Arsk : This module of ARS is the real first step to the radiative quantities calculation. It computes gaseous absorption coefficients on the specified resolution grid using all the spectroscopic parameters calculated by Arshls and interpolates absorption coefficients for any temperature and pressure profile defined by the user. The outputs of this package are used by next module.

¹Local Thermodynamical Equilibrium: In thermodynamics, a thermodynamic system is said to be in local thermodynamic equilibrium when it is in thermal, mechanical, radiative and chemical equilibrium.

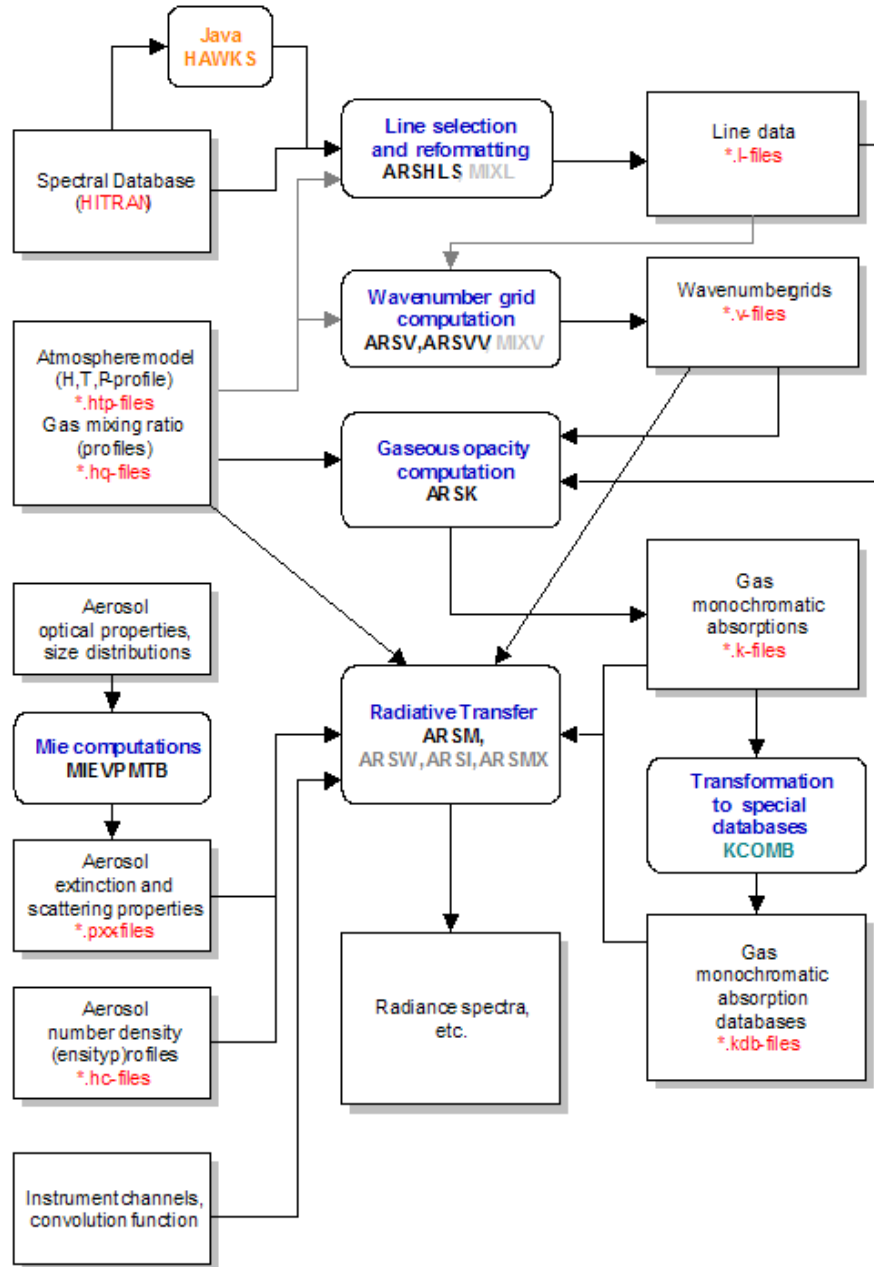


Figure 3.1: *ARS complete packages scheme. The code computes an exact line-by-line calculation for absorption and opacity of the gases.*

Arsm : Is the main package of ARS. It handles all the monochromatic quantities calculated by Arsk (and Arshls) and solves the radiative transfer equation under different condition as said before. In particular it calculates transmittance, radiance and fluxes inside and outside the atmosphere taking into account for single and multiple scattering both. The diffusion and emission of the aerosols and the presence of clouds are take into account also in this step. Many other parameters are considered here like observation geometry, solar radiance speci-

fication, surface properties, optical properties of aerosols, etc.

Mievpmtb : It is responsible for the aerosols optical properties calculations. Taking into account the right contribution of the aerosols to the radiative quantities requires aerosol properties parameters. Initialization files with extinction, single scattering albedo and coefficients in Legendre polynomial expansions of phase function as functions of wavenumber are needed. Using the MIEV0 [89] package based on Mie theory, this package provides such files from complex refractive index and parameters of aerosol particle size distribution for several commonly used size distributions.

After a briefly description of the software, the role of every single package and how they work together to obtain the final spectra is presented.

3.2.1 High resolution spectra

To obtain the synthetic spectra a number of steps are needed. In this paragraph the theoretical formulations of the physical parameters and how the software handles them are shown.

Absorption coefficient

First step is the extraction of some important spectroscopic parameters from a database. ARS was designed to work mainly with HITRAN (HIGH-resolution TRANsmission of molecular absorption) [64]. Basically is a data archive where informations on molecular spectral lines are stored in.

Arshls extracts those lines data from it and converts them into a reduced format. Moreover, it is possible to work with others HITRAN-like databases also, if they have a similar data format.

Before extracting lines data, the user can define many parameters as lines's intensity, line width and the shape of the line, the isotopes (if any), a different broadening (non-terrestrial atmosphere), wings line and/or wicked lines cutoff.

In detail, the quantities taken by **Arshls** from the database for every single line are:

- ν_0 : central position of the line in $[cm^{-1}]$ and atmospheric standard conditions: $T_0 = 296K$, $p_0 = 1 atm = 101325Pa$.²
- $S(T_0)$: line intensity at temperature T_0 in $[K]$
- $\alpha_{air}(p_0, T_0)$: selected gaseous molecule broadening due to the atmospheric environment.
- $\alpha_{self}(p_0, T_0)$: selected gaseous molecule broadening due to itself.
- E'' : transition lower state energy in $[cm^{-1}]$
- m : exponential index HWHM Lorentz's line shape vs. temperature ratio.

²All the HITRAN data are calculated and reported at these Earth standard conditions.

From those informations, the absorption of gaseous species can be computed. The absorption coefficient is the final output parameter of the **Arsk** package. It works on the grid created by the user with **Arsv** witch creates an optimized wavenumber grid according with positions, widths and strengths of the lines. **Arsk** takes into account different steps before coming to the final gaseous absorption coefficient.

The mathematical expression for the line intensity is defined as follow:

$$S(T) = S(T_0) \frac{Q(T_0)}{Q(T)} \exp \left[-c_2 E'' \left(\frac{1}{T} - \frac{1}{T_0} \right) \right] \frac{1 - \exp(-c_2 \nu_o / T)}{1 - \exp(-c_2 \nu_o / T_0)} \quad (3.1)$$

where:

$S(T_0)$ is the line strength at standard temperature condition.

$Q(T)$ is the full ³ statistical partition sum.

T is the air profile temperature defined by the user.

The constant $c_2 = hc/K_b$ with c speed of light and K_b Boltzmann's constant.

The molecular absorption cross-section in cm^2 per molecule in a spectral line with Voigt line shape is given by the formula:

$$\sigma_\nu = \frac{Sa}{\pi^{3/2}\beta} \int_{-\infty}^{+\infty} \frac{\exp^{-t^2} dt}{a^2 + (x - t)^2} \quad (3.2)$$

with

$$a = \frac{\alpha}{\beta} \quad x = \nu - \nu_0 \quad (3.3)$$

and where S is the line intensity, ν_0 is the line center, a is the Lorentz halfwidth, β is the Doppler halfwidth, which is defined as:

$$\beta = \frac{\nu_0}{c} \sqrt{\frac{2RT}{M}} \quad (3.4)$$

where R is the universal gas constant, T is the temperature, and M is the molecular weight in $[g/mole]$ of the gas.

Using special interpolation procedures [86] [46] and integrating over the t variable, the cross section can be so calculated.

Once (and if) Lorentz half width $\alpha(p_0, T_0)$ at the pressure p_0 and temperature T_0 is known, then for other pressures and temperatures it can be computed by the formula:

$$\alpha(p, T) = \alpha(p_0, T_0) \frac{p}{p_0} \left(\frac{T_0}{T} \right)^m \quad (3.5)$$

where m is a parameter particular for each individual line ⁴. It should be noticed that the previous formula for the Lorentz line half width includes both air- and self-broadening, the rigorous expression should be written as:

$$\alpha(p, T) = (\alpha_{air}(p_0, T_0)(p - p_s) + \alpha_{self}(p_0, T_0)p_s) \frac{1}{p_0} \left(\frac{T_0}{T} \right)^m \quad (3.6)$$

³Rotational and vibrational energy contributions are here included both.

⁴When the collision cross-section does not depend on temperature, the theory gives $m = 0.5$. In practice, m is slightly different and the difference in the broadening conditions on the Earth and other planets should be taken into account.

Even if this is the right expression one should take into account, the code uses the previous one for simplicity. The reason lies in the weight that partial pressure has to the final spectra. Especially for trace gases the corrections due to the p_s are small so that pressure line shift can be ignored.

At this point, it is clear the name *line by line* of this spectral technique.

This computational method sums the contributes of all lines for each wavenumber and the total opacity produced by all the lines is equal to the sum of the individual line opacities:

$$\sigma_\nu = \sum_i \sigma_{\nu i} \quad (3.7)$$

from this relation the absorption coefficient can be easily obtained as:

$$k_\nu = \sigma_\nu n \quad (3.8)$$

where $n = p/K_b T$ is the number density coming from the perfect gases equation of state.

It is important to notice that the absorption data witch are stored by **arsk** program in the output file are obtained per unit path length and for 100% pure gas.

Optical depth

To describe the extinction of a beam of radiation crossing an homogeneous atmospheric layer dl with an incidence angle $\cos \theta$, we have defined the optical depth.

Once divided for $\cos \theta$, this quantity can be interpreted as the average number of interactions with matter of a photon with wavenumber ν crossing the depth dl .

The expression for a single uniform cell of gas of length dl is:

$$d\tau_\nu = k_\nu^l(l) q(l) dl \quad (3.9)$$

In formula, optical depth is the integral of k_ν times the mixing ratio ⁵ $q(l)$ along the vertical axis or the line of sight depending on the particular consideration.

One of the main assumption in atmospheric science is to consider for sake of simplicity the atmosphere as composed of a finite number of plane and parallel layers each with uniform temperature and pressure in its interior. At the radiation crossing between the levels $l_0 = 0$ and $l_1 = z_1$ is associated an optical depth of:

$$\tau_\nu = \int_{l_0}^{l_1} k_\nu^l(l) q(l) dl \quad (3.10)$$

Therefore optical depth is the integral calculated along the line of sight of absorption coefficient k_ν^l multiplied by the mixing ratio $q(l)$.

⁵The mixing ratio is the molar concentration over the total amount of atmospheric gas for each point. It is defined as the ratio between the number of molecules of the generic gas and the total number of molecules of all the atmosphere.

Transmittance

It is now possible to calculate the attenuation of the radiation along the line of sight. Transmittance is simply the exponent of the optical depth:

$$t_\nu = \exp \left(\frac{\tau_\nu}{\cos \theta} \right) \quad (3.11)$$

In the solar region, we often deal with the total transmittance of the atmosphere from the space to the surface and back:

$$t_\nu = \exp \left[-\tau_\nu \left(\frac{1}{\cos \theta_0} + \frac{1}{\cos \theta} \right) \right] \quad (3.12)$$

where τ_ν is the total optical depth in the nadir (strictly vertical) direction, θ_0 is the sun zenith angle and θ is the line of sight zenith angle.

Radiative Transfer without scattering

If the effect of aerosols is negligible, in **Arsm** package the Radiative Transfer Equation for the thermal emission considering a plane parallel atmosphere in local thermodynamic equilibrium, is calculated as the integral of the Planck function on transmittance (which depends on altitude) from the bottom level (or a reference altitude) to the top of the atmosphere, plus an additional term taking into account for surface emission.

A nadir viewing instrument would see the upward monochromatic radiation intensity as:

$$I_\nu = \varepsilon_\nu B_\nu(T_0) \exp \left[-\frac{\tau_{max}}{\cos \theta} \right] + \int_0^{\tau_s} B_\nu(T(\tau_\nu)) \exp \left[-\frac{\tau_{max}}{\cos \theta} \right] d(\tau_\nu / \cos \theta) \quad (3.13)$$

or, in equivalent form:

$$I_\nu = \varepsilon_\nu B_\nu(T_0) t_{\nu,0} + \int_0^{t_0} B_\nu(T(\tau_\nu)) dt_\nu \quad (3.14)$$

This last expression can be seen as composed by two terms: the emission from the bottom level (surface or equivalent altitude) ε_ν , attenuated by all the layers above it (first term) and the total contribution of all the other layers (second term). The integral over the transmittance of all the atmosphere in the second term means that every layer emits thermal radiation absorbed by all the overlying layers.

In the near infrared, where the solar radiation dominates, the radiance is simply the solar radiation flux F_ν^0 outside the atmosphere (divided by π) times total atmosphere transmission, with account for the surface albedo a_ν :

$$I_\nu = \frac{F_\nu^0 \cos \theta}{\pi} a_\nu \exp \left[-\tau_\nu \left(\frac{1}{\cos \theta_0} + \frac{1}{\cos \theta} \right) \right] \quad (3.15)$$

In principle, is possible to obtain the atmospheric outgoing radiation from the direct integration of the previous relations if the thermal and the species concentration profiles as function of altitude are known.

Radiative Transfer with multiple scattering

Actual atmospheres are not only a mixture of molecules in gaseous phase. Particles of different size, shape, composition and lifetime substantially modify the spectral behavior observed by any instrument. In order to obtain physical informations under more realistic condition from spectral analysis, is very important to simulate the presence of aerosols and particles in the atmosphere almost always.

From a mathematical point of view, the presence of aerosols changes the expressions of the radiation field emerging from a scattering atmosphere with new additional terms due to different aspects of the radiation itself.

Basically we can consider :

- all the photons which are emitted from the surface (or equivalent bottom level) in any direction and then send towards to the observer after a single interaction with the particles.
- all the photons which went towards multiple scattering events or diffusion of photons emitted by the atmosphere.

Previously, we have seen that the equations for radiative transfer in non scattering atmosphere are relatively simple. However, these equations are not applicable to the analysis of sunlight reflected by clouds in planetary atmospheres and are hence use only in the thermal IR spectra. Even in this case however, neglecting the scattering effects of atmospheric aerosols can sometimes lead to errors, especially if cloud particles are of a size approximately equal to or greater than the wavelength.

For particles that have non-negligible size compared with the wavelength calculation of the *extinction cross section* $\sigma_{\nu,ext}$, the *phase function* $P(\theta', \phi')$ and the *single scattering albedo* $\tilde{\omega}_{\nu}$ (see expressions (2.79), (2.68) and (2.86)), becomes more complicated.

However, provided the aerosols particles are spherical and that the complex refractive index $m=n+ik$ as a function of wavelength is known, Maxwell's equations may be solved analytically by the Mie theory to calculate the scattering properties.

For solving the atmospheric radiative transfer equation, we need only to know the three previous quantities $\sigma_{\nu,ext}$, $P(\theta', \phi')$ and $\tilde{\omega}_{\nu}$.

The quantity $P(\theta', \phi')$ for spherical particles can be calculated with Mie theory but do not have a simple analytical expression. However, it is sometimes useful to have a more simple parameterized form of the phase function to use in the modes that can reasonably well approximate real phase functions of particles.

One such representation is the *double Henyey–Greenstein function*. All these modifications to the radiative transfer equation, greatly increase the computation time and thus scattering calculations are notoriously difficult and slow.

Moreover the aerosols extinction crossing section, even if not dependent on temperature, has very complicate relation on the particles size and their complex refractive indexes.

For these reasons usually the problem is solved using numerical models which approximate the continuum radiation field present in the atmosphere with a finite number of streams along some fixed directions.

In the ARS code the task of the treatment of scattering is faced with different ap-

proaches.

The possible options are:

- Black aerosols approximation: absorption is simply added to the gaseous absorption. This condition is almost valid for thermal part of the electromagnetic spectrum but absolutely not for solar part.
- Two stream approximation: the code estimates the multiple scattering part of the source function as average values on two hemispheres only. The source function is then integrated to give the intensity of outgoing radiation. We can have three options for the fluxes:
 - Fluxes are evaluated with TWOSTR code [19].
 - Fluxes are evaluated using layer flux adding procedure similar to Modtran 3 code [76].
 - Fluxes are evaluated using a combination of the previous ones. The first for thermal emission and the second for the solar radiation (however, this option is implemented only together with the Correlated-I correction).
- Discrete ordinate method: the code estimates the multiple scattering using DISORT (Discrete Ordinate Radiative Transfer) code [54] [55].
- Correlated-I correction: this approach provides the spectrum almost coinciding with that given by DISORT, but in hundreds times faster [69].
- SHDOMPP code [56].

We always performed an exact line-by-line computation, without any approximations. Many Radiative Transfer codes, especially for Earth atmosphere, as FASCODE or LBLRTM, have many special short cuts, which give ready approximate solutions for fast simulations of transmission and radiance spectra.

As black boxes, they give ready solutions but are not flexible due to the unknown details of their options and code internal computations. In general they increase performance but reduce precision.

For this reason, even if line-by-line method is not very fast (in computations of gaseous opacity and simple spectra) with respect to other codes, this slower but more robust approach was preferred.

Technically, in our simulation radiative transfer for multiple scattering is computed using mainly TWOSTR for the thermal fluxes and MODTRAN 3 with the adding layers procedure for the solar fluxes. From Mie theory a complete phase function (with all *Legendre polynomials* calculations) and a Heney-Greenstein phase function are used.

Solar spectrum

In order to reproduce the level of VIMS in radiance units [$\text{erg cm}^{-2} \text{s}^{-1} \text{sr}^{-1} \text{nm}^{-1}$], the solar spectrum for the region between near $1 \mu\text{m}$ and $3 \mu\text{m}$ has to be included. Many authors provided different solar spectra both at low resolution [15] and high [8] resolution.

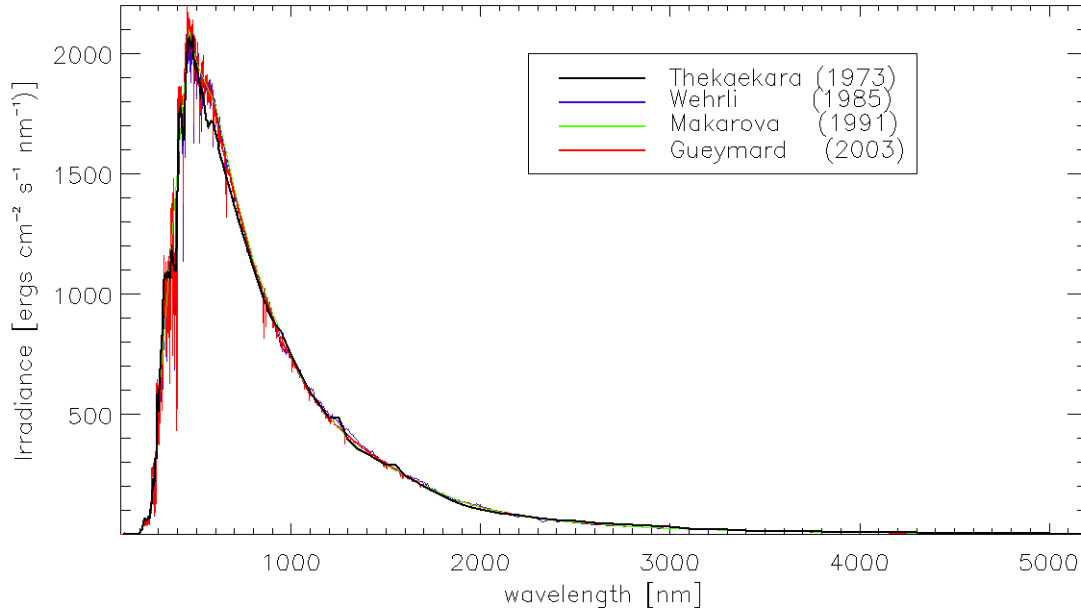


Figure 3.2: *Solar spectrum as recorded by different instrument at very different resolutions. For coherence we use the spectrum of Thekaekara, the same used in the instrument calibration pipeline.*

Because we will match the synthetic spectra with the instrumental ones, for coherence we adopt the same solar spectrum file used in the calibration pipeline of VIMS data cubes [88]. This spectrum is used for all the simulations. In figure 3.2, different resolution solar spectra are shown.

Instrumental convolution

In order to compare the synthetic spectra with the observed ones, a convolution on the instrumental grid at its spectral resolution is needed.

The equation used by the package is:

$$I(\nu) = \int I_{\nu'} \Phi(\nu - \nu') d\nu' \quad (3.16)$$

where $\Phi(\nu - \nu')$ is the instrumental function. The same relation is used to convolve not only radiance but other quantities as transmittance and reflectance as well.

All the convoluted spectra are expressed in wavenumber units so that this last option is useless when the observed spectra are in wavelengths units.

Image spectrometer data are usually measured in wavelength units.

We shall see in the paragraph dedicated to the convoluted spectra how this problem has been solved.

However, convolution is the final step of **Arsm**.

3.3 Atmospheric model

Elemental abundances in planetary atmospheres provide useful information pertaining to questions about planet composition, formation, and evolution.

The importance of relative enrichment of the elements in the atmospheres of the planets is vital to constrain formation and evolutionary theories of the entire solar system.

In the Giant Planet case, bulk composition retains the chemical signatures of the primordial solar nebula from which these planets formed, although significantly reprocessed by accretion, thermochemistry, photochemistry and gravitational differentiation over the intervening eons [41].

Many questions, about the mass of rocky or icy material attained by Saturn during its accretion; the size and composition of Saturn's core and degree of homogenization with the extended molecular atmosphere; the possible sources of material and the temperature of their formation incorporated into Saturn; the possible timescales for the formation of Jupiter and Saturn; the thermochemical pathways and cooling history of the planet in the billions of years since its formation, and many other questions, are directly related to the elemental abundances knowledge.

The entry probe of *Galileo* mission at Jupiter provided informations of bulk composition down to the 20 *bar* level, but unfortunately in the case of Saturn our knowledge of its heavy element enrichment is restricted to those accessible from infrared remote sensing. However, even if it is possible to obtain abundances remotely through optically active molecules, the only way to address realistic values of abundances in Giant Planets is by probe.

The material intrinsic to Saturn is further modified by the influx of other material as ring particles, dust, micrometeorites, satellite debris and other material sources, into the high stratosphere.

The rate of influx and the longterm consequences of the presence of external species on the atmospheric chemistry are yet to be investigated.

In addition to bulk composition, the relation between radiative climate influences, photochemistry and the spatial and temporal distribution of Saturn's rich collection of hydrocarbons is poorly understood, requiring to constrain their horizontally and vertically distribution and in photochemical modeling to assess the relative influences of photochemistry, atmospheric transport, and shielding due to the uncertain properties of Saturn's aerosols distribution.

The same is true for photochemical destruction of tropospheric compounds particularly and their relation to tropospheric clouds opacity, whose latitudinal distributions indicate variability in the photochemical lifetimes at different latitudes.

With a composition similar to the Sun, the Giant Planets atmospheres are mainly composed of molecular hydrogen (H_2) and helium (He).

The solid core of both Jupiter and Saturn accounts for about 10% of the mass of the planets, making it mostly liquid and gassy. The composition of this gassy and icy makeup of their atmosphere contains significant amounts of other molecules.

Before 1970 only H_2 , CH_4 and NH_3 had been positively identified in Giant Planets atmosphere. Today, the number of known species is ten times greater.

As minor constituents, the bulk of the atmosphere of Saturn contains methane (CH_4), methane deuterate (CH_3D), ammonia (NH_3), water (H_2O), phosphine (PH_3), hydro-

gen sulfide (H_2S), carbon monoxide (CO), carbon dioxide (CO_2), germane (GeH_4) and arsine (AsH_3). Moreover, there is evidence for the presence of HF , HCl , HBr and HI .

The chemical composition in turn affects many physical aspects of the atmosphere such as its thermal structure, radiation balance, dynamical processes, ionospheric structure, and the formation of clouds and hazes. The upper atmospheric photochemistry of is reasonably straightforward because methane alone of all the major atmospheric constituents is volatile enough and abundant enough on the outer planets that it can diffuse or be dynamically injected into the upper atmospheres where it can interact with solar and corpuscular radiation and instigate photochemistry.

In the stratosphere of Saturn in fact, several hydrocarbons have been detected. From the photodissociation of methane spectral signatures have been found for CH_3 , C_2H_2 , C_2H_4 , C_2H_6 , $\text{CH}_3\text{C}_2\text{H}$, C_3H_8 , C_4H_2 and C_6H_6 [80].

Assuming cosmic abundances, it is possible to estimate for the Giant Planets the expected enrichment in heavy elements with respect to hydrogen [82].

With the assumptions that all heavy elements are equally trapped in ices and following the infall of the protosolar gas and the subsequent heating of the protoplanets, all elements are uniformly mixed in the interiors, the expected enrichments in heavy elements for the giant atmospheres can be calculated and compared with the observed ones.

From the absorption signatures observed both in solar and thermal part of planetary spectra, compositional informations can be obtained by the column density of an atmospheric constituent. In particular, the $5\ \mu\text{m}$ region allows the determination of the abundance of several minor compounds in Giant Planets atmospheres.

These kind of measures allow to determine abundances and mixing ratios⁶.

Only in Jupiter case, *in situ* mass spectrometry measurements have provided a major contribution about the composition of the neutral atmosphere of the Jovian atmosphere, thanks to the Galileo probe which entered the planet on December 7, 1995.

In the first comprehensive thermochemical-equilibrium calculations for Saturn, the large background atmospheric H_2 abundance allows CH_4 to be the dominant carbon-bearing molecule throughout Saturn's atmosphere, with all other carbon species having abundances much less than methane [23]. Methane is expected to be well mixed in all the atmosphere.

The same model predicts on Saturn, the formation of P_4O_6 in vapor phase formed from the oxidation of phosphine by water. These molecule is expected to be the thermodynamically stable form of phosphorus in the deeper levels of the atmosphere between $400\ \text{K}$ and $900\ \text{K}$ region, with PH_3 becoming dominant only at deeper levels for temperatures in excess of $1000\ \text{K}$.

At temperatures below $400\ \text{K}$ the P_4O_6 vapor is expected to be converted to a solid $\text{NH}_4\text{H}_2\text{PO}_4$ condensate, and gas-phase phosphorous-bearing species are expected to have low abundances in the upper troposphere of Saturn under thermochemical-equilibrium conditions [29].

Carbon monoxide is expected to have an exceedingly low abundance in the observ-

⁶Being hydrogen the main element of the atmosphere of the Giant Planets, often the abundances of the species are relative to H_2 , in order to facilitate comparison to the solar values. Mixing ratio is the ratio between the number density of a specie over the H_2 number density.

able regions of the upper troposphere but becomes more and more abundant with increasing temperature and depth.

The dominant forms of oxygen, nitrogen, and sulfur throughout the thermal structure found in Saturn's troposphere are H_2O , NH_3 and H_2S .

The lack of any appreciable signatures of some molecules in different spectral ranges of the observed spectra, has strongly suggested that some species are severely depleted in Saturn's upper troposphere.

Previous spectra of Saturn have been recorded in the thermal range and with respect to atmospheric composition, a number of different results have been published.

Vertical abundance of NH_3 has been retrieved by many authors [60] showing the evidence for a strong depletion above the 1.2 *bar* level.

The phosphine is not in thermochemical equilibrium at the cold temperatures and low pressure which it is observed [6]. Vigorous vertical eddy mixing creates a significant abundance in the observable troposphere between 100 *mbar* and 800 *mbar* transporting this trace gas to high altitudes faster than it can be decomposed chemically. Moreover, the chemistry of PH_3 also allows us to use the upper tropospheric measures to probe the equilibrium composition of Saturn's deep atmosphere [63].

Evidence of vertical abundance of H_2O in upper troposphere has been investigated by other studies [3].

For all these trace gases, many models use saturation profiles to estimate the numerical constraints in which the abundances are embedded in.

Even in minor percentage, all the chemical constituents mentioned before are direct responsible for the spectral behavior observed on Saturn.

3.3.1 Gaseous species

In order to simulate the atmosphere of Saturn, our model takes into account the main molecules which the atmospheres of Giant Planets are made of.

The atmosphere is modeled as a mixture of eight different gases: CH_4 (considering separately its three isotopes $^{12}\text{CH}_4$, $^{13}\text{CH}_4$, CH_3D), H_2O , NH_3 , PH_3 .

H_2 and He has been also considered to define the *continuum* level of IR emission. All these species are spectroscopically and optically active in the bandwidth of the instrument.

The mixing ratios of the considered species are constant in altitude, with the exception of NH_3 , PH_3 and H_2O as mentioned before.

Figure 3.3 shows the mixing ratio versus pressure plot of the profiled gases, while the others are maintained constant along all the atmospheric layers and their values are shown in Table 3.1.

A constant value of $\chi_{\text{CH}_4} = 4.4 \cdot 10^{-3}$ for CH_4 mixing ratio is adopted, this value has been retrieved by other studies [82]. Different authors [37] assume a value of $\chi_{\text{CH}_3\text{D}} = 3.4 \cdot 10^{-7}$ for deuterate methane in Saturn's atmosphere, the same value is adopted in our model. For the NH_3 and PH_3 profiles, the data are taken from Cassini - CIRS observations [63]. These authors profile the phosphine mixing ratio as a constant value of $\chi_{\text{PH}_3} = 5.3 \cdot 10^{-6}$ for levels deeper than 500 *mbar* decreasing with a mean scale height. For the ammonia a similar profile has been adopted with a value $\chi_{\text{NH}_3} = 1.1 \cdot 10^{-4}$ for depths below ~ 1.4 *bar* level.

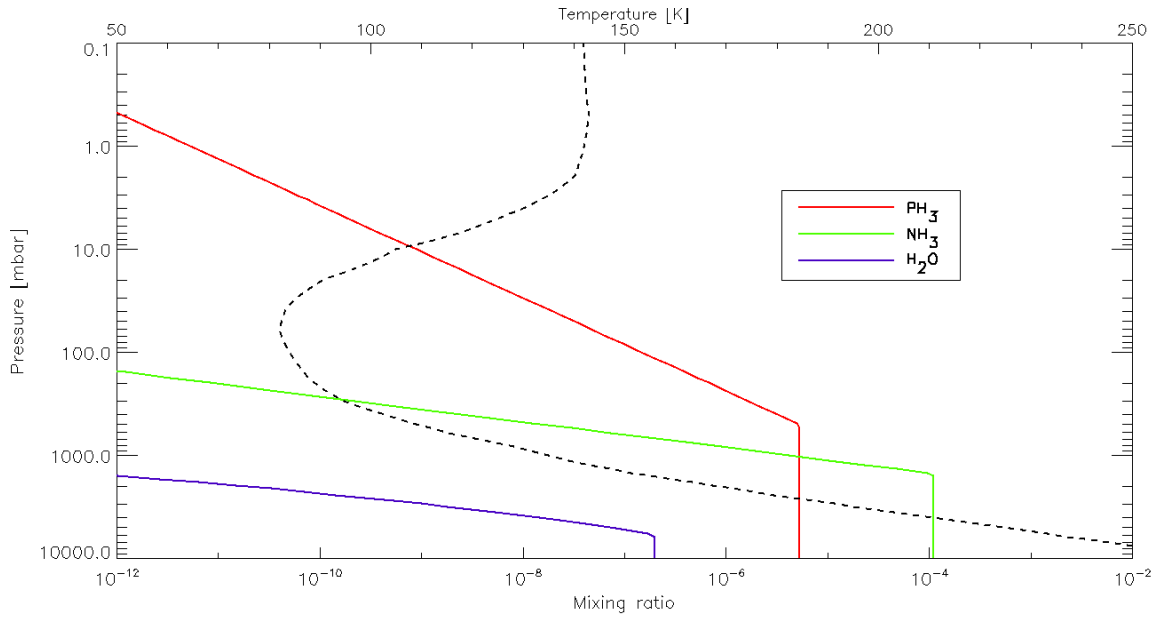


Figure 3.3: *Profiled species for Saturn's atmosphere. In dashed line the pressure-temperature profile is also shown.*

The water profile has been created using the saturation curve for water [2], using 1% of relative humidity until the value of $\chi_{\text{H}_2\text{O}} = 2 \cdot 10^{-7}$ adopted by other authors [3], then the deep mixing ratio remains constant for all the thermal profile.

Molecular hydrogen and helium are the most abundant constituents in the upper atmospheres of Giant Planets.

In Saturn atmosphere, the percentages of these two constituents are $\sim 96\%$ (H_2) and $\sim 4\%$ (He), being all the other species in trace.

Whereas the high proportion of hydrogen gas can be directly detected from its absorption spectrum, percentages of helium in each gas giant are extrapolated from the assumption that nearly all of the remaining gas (albeit nearly impossible to identify directly) is He, in nearly solar abundances.

After the Voyager mission, a value of $\chi_{\text{He}} = 0.034$ was retrieved [25].

A reanalysis by the same authors of the Voyager radio occultation profiles however, gives a new value of mixing ratio for helium [26]. Using these new percentages, we assume in our model a constant value of $\chi_{\text{H}_2} = 0.963$ for hydrogen and $\chi_{\text{He}} = 0.118$ for helium.

3.3.2 Thermal profile

The first spacecraft observations of Saturn's thermal structure came from Pioneer 11 in 1979. From the inversion of infrared measurements at $20 \mu\text{m}$ and $45 \mu\text{m}$, temperatures from 60 mbar to 500 mbar were retrieved for the Saturn upper atmosphere [42]. More extensive thermal data were obtained by the infrared spectrometer IRIS on Voyagers 1 and 2. Voyager IRIS data were used to obtain meridional temperature

Molecule	Mixing ratio
[H ₂]	0.963
[He]/[H ₂]	0.118
[CH ₄]/[H ₂]	4.4 e-3
[CH ₃ D]/[H ₂]	3.2 e-7
[PH ₃]/[H ₂]	profiled
[NH ₃]/[H ₂]	profiled
[H ₂ O]/[H ₂]	profiled

Table 3.1: *A priori* mixing ratio values. Mixing ratio are given relative to H₂, only hydrogen value is referred to the total atmosphere.

profiles at three pressure levels in the upper troposphere just after northern spring equinox [14].

Other studies have retrieved profiles in different times covering different regions of the planet, many data come from a variety of instruments, including ground based telescopes and space satellites.

Measures from Infrared Space Observatory (ISO) [66] provided other data [49] for the thermal structure of Saturn, especially for the stratosphere [87].

Measures of southern hemispheric temperatures from Cassini-CIRS data were presented [40]. Temperatures from CIRS mapping observations were retrieved by other authors [62], giving a latitude pressure cross section of temperatures in the upper troposphere and middle stratosphere during southern mid-summer.

There is a well-defined tropopause at 80 *mbar*, separating a strongly statically stable stratosphere with temperatures increasing with altitude, from a troposphere with temperatures increasing with depth. In the upper troposphere, the temperature gradient increases with depth down to approximately 500 *mbar*, where the gradient becomes nearly dry adiabatic.

This transition to the adiabat likely indicates the radiative-convective boundary, with temperatures and dynamics at higher pressures determined primarily by convection, and the temperatures at lower pressures determined by solar heating and the solar driven circulation.

In order to define the spectroscopic model for the generation of synthetic spectra, the first task is to specify a self-consistent pressure-temperature profile for the atmosphere of Saturn.

As a starting point we adopted one of the profiles used for the analysis of the Cassini-CIRS data [16]. This profile is able to reach only the 4 *bar* level. The temperatures at pressures larger than about 4 *bar* have been obtained by extrapolation of this temperature profile according to a dry adiabatic.

Figure 3.4 shows both of the retrieved profiles from different observations and the profile used in our model.

An interpolation on these data has been made in order to model the Saturnian atmosphere as a stack of homogeneous layers. Assuming the usual *plane-parallel* condition, the atmosphere has been split in 150 layers with a constant layering step of 5 *Km*, assuming constant, inside every single layer, all the physical parameters. The pres-

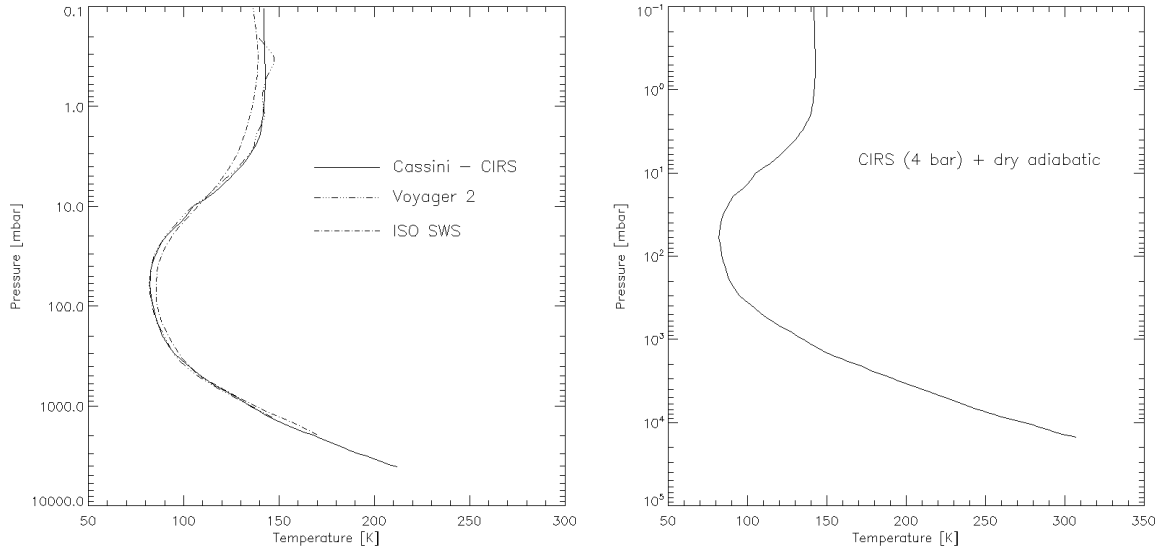


Figure 3.4: *On left, pressure-temperature profiles retrieved by different instruments. The Cassini-CIRS profile reaches the 4 bar level. On right, the thermal profile used in this work, obtained from the Cassini-CIRS profile with an adiabatic extrapolation to the 15 bar level.*

sure covers the range between 0.05 *mbar* and 15 *bar* and the temperature between 82 *K* (tropopause) and 306 *K* for a total height of 745 *Km*. For reference, the 1 *bar* level is the zero of the altitudes, with the top of the atmosphere at 515 *km* and the bottom at -230 *km*.

3.4 Synthetic spectra

Before going on to look at the spectroscopic model and all the quantities which will generate synthetic spectra used for this work, we will briefly look at the spectrum of Saturn in the instrument bandwidth spectral range.

Overview of Saturn's near-IR Spectrum

Saturn's near-IR spectrum is characterized by spectral signatures of different species. If expressed in wavenumber units, VIMS-IR bandwidth covers the range between near 1880 cm^{-1} and 10⁴ cm^{-1} .

As shown in Figure 3.5, NH_3 and PH_3 are the main responsible for the thermal absorption near 2000 cm^{-1} , where the Planck's curve decreases.

In the range between 2000 cm^{-1} and near 3600 cm^{-1} two prominent windows centered at about 3225 cm^{-1} and 3545 cm^{-1} are well visible. These highly transmissive spectral regions straddle the strong absorption CH_4 band centered at 3018 cm^{-1} and some weak PH_3 bands lying mainly in the region between 3300 cm^{-1} and 3600 cm^{-1} [35]. In the region between 3200 cm^{-1} and 3300 cm^{-1} , weak features of ethane (C_2H_6) are

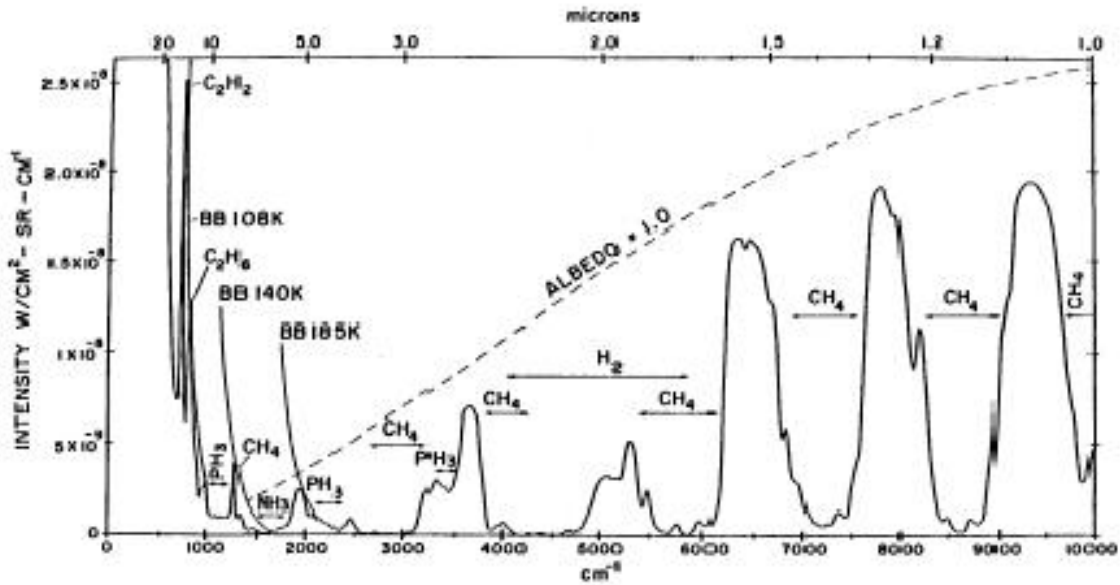


Figure 3.5: Saturn's nearIR radiance spectrum. The main molecules and the respective absorption features are also shown [35].

interspersed.

In the range between 3550 cm^{-1} to 3750 cm^{-1} no absorption occurs.

Molecular hydrogen and CH_4 both absorb from about 3800 cm^{-1} to 4800 cm^{-1} . In this range, strong overtone and combination bands of methane occur at 4223 cm^{-1} , 4340 cm^{-1} and 4540 cm^{-1} , where in addition to the H_2 fundamental absorption band, they totally darken the planet from 4100 cm^{-1} to 4600 cm^{-1} .

Near 4750 cm^{-1} the radiance level is again zero, owing mainly to the Q(1) component of H_2 absorption.

Additional but negligible CH_4 opacity from approximately 4800 cm^{-1} to 4950 cm^{-1} are also present. In the region between 4800 cm^{-1} and 5000 cm^{-1} , the increasingly transmissive H_2 produces a nearly constant-slope *continuum*.

Several CH_4 bands of varying strengths modulate the absorption band between 5000 cm^{-1} and 6000 cm^{-1} .

A moderately strong CH_4 feature is at 5200 cm^{-1} with a measurably weaker one adjacent to it at 5300 cm^{-1} . Other methane bands lie at 5400 cm^{-1} , 5600 cm^{-1} and near 5850 cm^{-1} and by 5400 cm^{-1} the H_2 *continuum* has recovered fully.

Finally, strong and intense CH_4 absorptions bands centered around 7200 cm^{-1} , 8600 cm^{-1} and 9900 cm^{-1} shape the remaining portion of the spectrum.

3.4.1 Spectroscopic model

In order to make use of the definitions previously alluded to, a systematic plan must be developed which will lead to the generation of synthetic spectra.

The first step using a line-by-line code is the choice of the grid for the simulation. This is a very important step, being computation time dependent on chosen resolu-

Molecules	$^{12}\text{CH}_4$, $^{13}\text{CH}_4$, CH_3D , NH_3 , PH_3 , H_2O , H_2 , He	units
Wavelength range	1000 ÷ 5200	[nm]
LBL wavenumber range	1880 ÷ 10000	[cm^{-1}]
LBL resolution	0.1	[cm^{-1}]
Lineshape	Voigt profile (broadening correction)	-
Wings cutoff	500	[cm^{-1}]
LBL grid points	81200	-
VIMS channels	256	-
Gaussian FWHM	~ 19.0	[nm]

Table 3.2: Main parameters of the spectroscopic model used to generate synthetic spectra.

tion. The choice of the step of the initial wavenumber grid is directly related to the final appearance and quality of the synthetic spectra.

Remembering the expression (2.11) for the absorption coefficient and the related line shapes described in the previous chapter, low atmospheric pressure produces thin lines in the spectrum. For this reason, to properly simulate it, it's needed a monochromatic grid with a very small step. On the other hand, when pressure becomes high the opposite is true, lines are much broadened and a wider monochromatic step is enough to compute the spectrum.

In order to reproduce the signal of the instrument, the wavenumber grid covers all the bandwidth, between 1880 cm^{-1} ($5.32 \mu\text{m}$) and 10^4 cm^{-1} ($1.0 \mu\text{m}$).

Some previous tests we have made, demonstrated that a constant wavenumber grid step of 0.1 cm^{-1} with a *wings cut-off* at 500 cm^{-1} from line center, were enough to ensure both behaviors. For calculation simplicity we did not take into account a different cut-offs with altitude. In Table 3.2, the main parameters are summarized.

With a total number of 81200 points, absorption coefficient for every species has been calculated on this wavenumber grid.

3.4.2 Absorption coefficients

After the definition of the molecules, their abundances, the thermal profile, the resolution of the grid and other parameters, we have run the code to generate the absorption coefficient of all the species involved.

The efficiency of calculations can be increased by the usage of various time-saving procedures as line selection, decomposition of the line profile, appropriate choice of the altitude and wave number mesh width, interpolation between levels in the thermal profile and many others, which are eventually adopted case by case if they do not produce important changes in the results.

To generate synthetic spectra we used the line list from the last version of HITRAN. As said before the ARS code uses the HITRAN database for all the spectroscopic parameters used in calculations. This database has been recently revised [64], with new molecular parameters. Many applications require reliable high-resolution methane

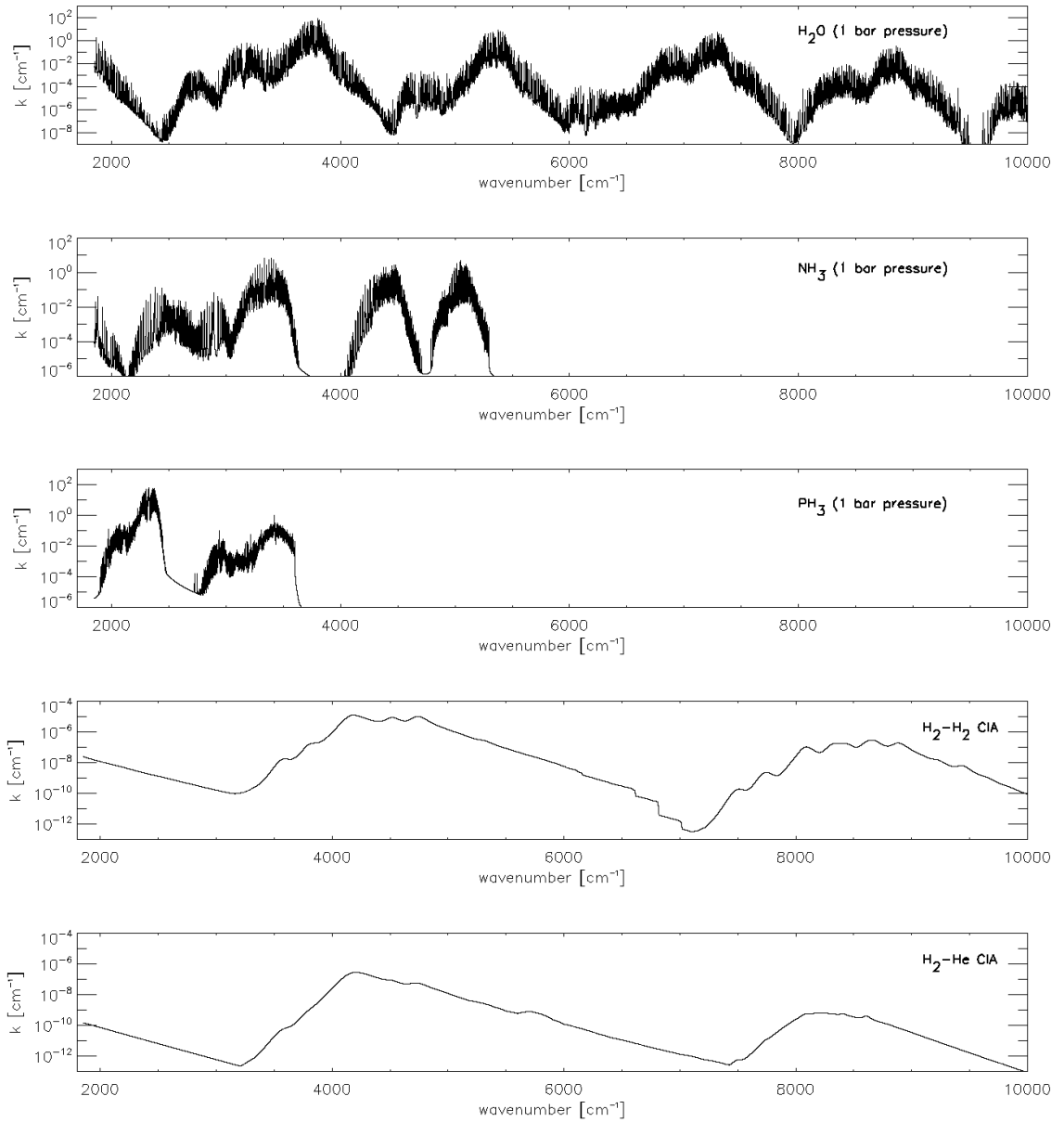


Figure 3.6: Absorption coefficient of H_2O , NH_3 , PH_3 and $\text{H}_2\text{-H}_2$, $\text{H}_2\text{-He}$ Collision Induced Absorption, calculated at 1 bar and 135 K on 81200 points of the monochromatic grid with a resolution of 0.1 cm^{-1} between 1800 cm^{-1} and 10000 cm^{-1} .

parameters throughout the spectrum. Besides being a major component of the Giant Planets and Saturn's large moon Titan, it is a prominent in the atmospheres of brown dwarf stars, and has recently been identified by in the atmosphere of exosolar planet as well [68]. Nevertheless, it is a greenhouse gas and absorber in the terrestrial atmosphere.

The total number of CH_4 lines are approximately $6 \cdot 10^4$ including very weak lines. In this last edition of the database, the parameters of $^{12}\text{CH}_4$ have been changed. Line

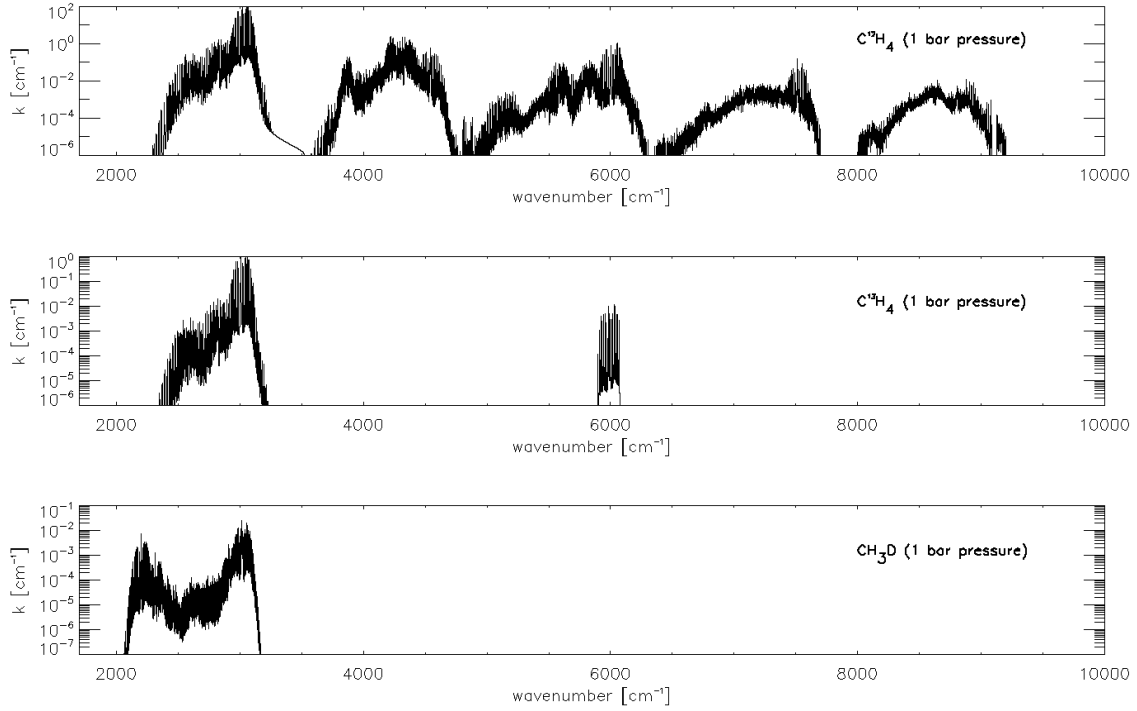


Figure 3.7: Absorption coefficients for $^{12}\text{CH}_4$, $^{13}\text{CH}_4$ and CH_3D at the same spectroscopic conditions of Figure 3.6.

positions and intensities were revised from 0 cm^{-1} to 3300 cm^{-1} using calculated values from the analysis for the three lowest polyads from the ground state. Few new bands of CH_3D were added, but no changes were made to the $^{13}\text{CH}_4$ parameters.

Phosphine is a significant contributor to the continuum opacity in the $5\text{ }\mu\text{m}$ window in the atmosphere of Giant Planets, which can be used as a means of probing the deeper atmospheric structure.

Spectral line parameters for new bands of PH_3 have been added in the region from 2724 cm^{-1} to 3602 cm^{-1} , based on recent studies [74].

In addition, the collision-broadened parameters of the previously existing data in HITRAN have been updated.

The available PH_3 line list however, only partially covers our range and also lacks line-by-line information for some PH_3 absorption near $3\text{ }\mu\text{m}$. Recent studies of PH_3 in fact, have confirmed the need to improve and normalize the calculated intensities for the bands at $5\text{ }\mu\text{m}$ and $3\text{ }\mu\text{m}$.

Water vapor spectroscopy is of importance to many applications. Not only are the spectroscopic parameters needed for studies of the climate and energy budget of the Earth, but also for the atmospheres of stars.

The recommended line list for water remains in a state of continued evolution. Substantial changes to the half-width parameters for the isotopologues and the addition of new data for isotopically substituted species are among the prominent recent modifications in the database. Being all the HITRAN molecular parameters referred to

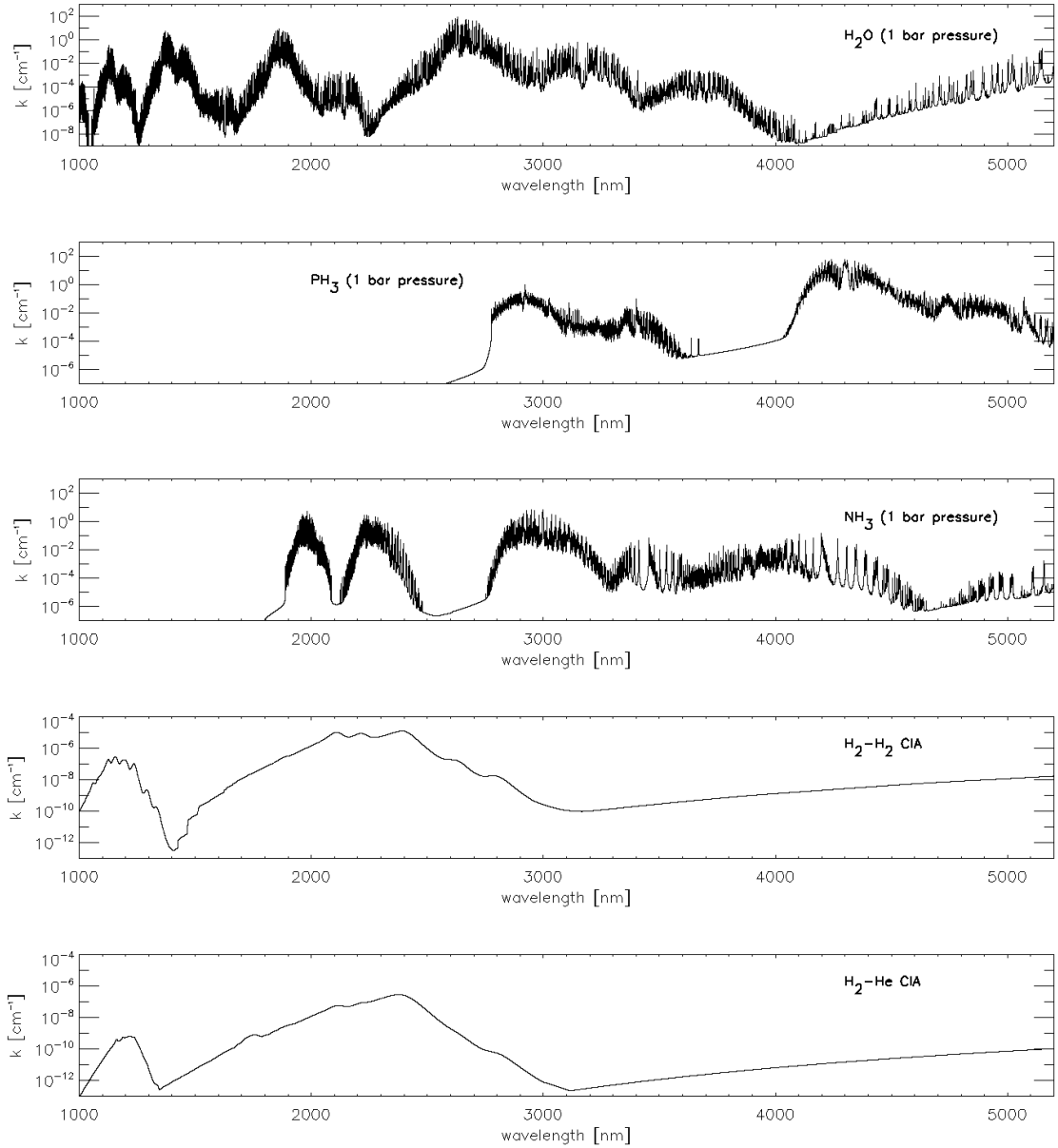


Figure 3.8: *Same absorption coefficients of Figure 3.6 but expressed in wavelength units covering the instrument bandwidth.*

the Earth's atmospheric conditions, the halfwidth in the database are related to the broadening due mainly by N_2 and O_2 .

A broadening correction was needed because the difference of the main atmospheric constituents, H_2 and He.

If we consider again expression (3.5):

$$\alpha(p, T) = \alpha(p_0, T_0) \frac{p}{p_0} \left(\frac{T_0}{T} \right)^m$$

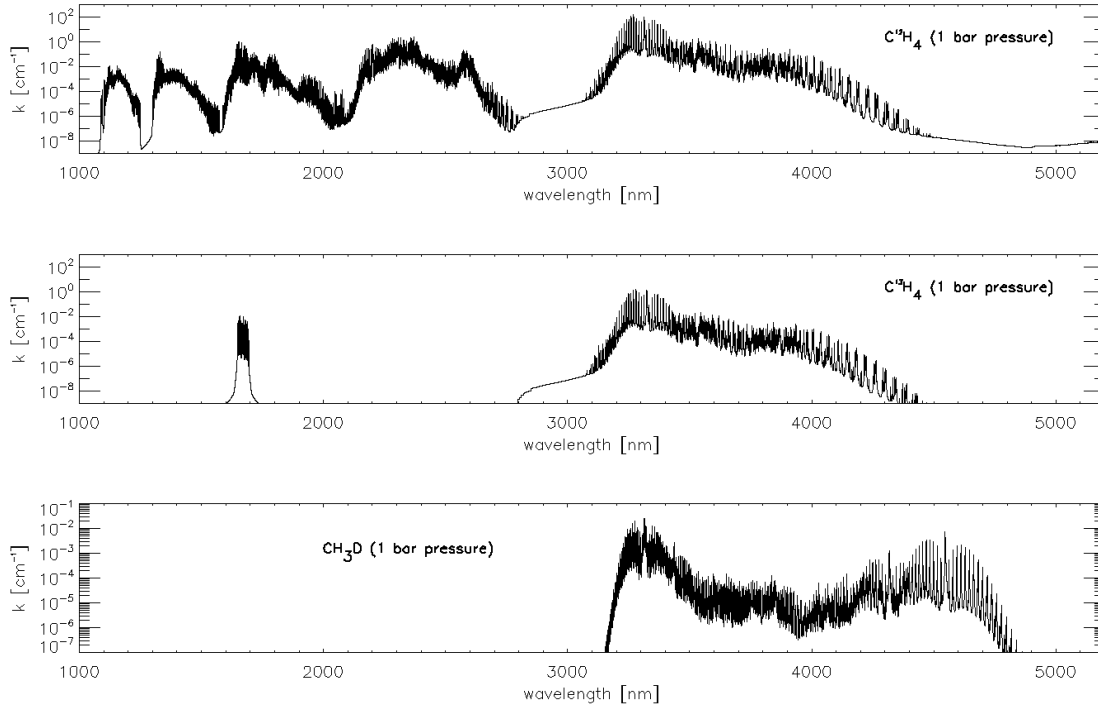


Figure 3.9: *Methane isotopes absorption coefficients on instrumental spectral range.*

for the broadening of a line due to the other molecules, for CH_4 a value of $\alpha_{\text{CH}_4}(p_0, T_0) = 0.0728$ has been set as linewidth with a value of $m = 0.5$ for the exponent, while for NH_3 , PH_3 and H_2O , $\alpha(p_0, T_0) = 0.075$ and $m = 0.83$ have been adopted.

In Figure 3.6, the absorption coefficient for H_2O , NH_3 and PH_3 are shown in wavenumber units. In Figure 3.7, methane isotopes absorption spectra are shown.

The *continuum* level

Collision Induced Absorption (CIA) due to hydrogen pairs has been recognized, for many years, to play an important role in the radiative transfer of atmospheres of all the outer planets and the study of collision-induced spectra for these interacting systems is, therefore, of considerable astrophysical interest.

It is well known that homonuclear diatomic molecule does not exhibit an ordinary vibration-rotation spectrum since it does not present a permanent dipole moment $\vec{M}$ to interact with the electric field vector $\vec{E}$ of the radiation.

The CIA absorption on the contrary, arises from transient dipole moments induced by intermolecular interactions [5]. The dominant induction mechanism is the polarization of the collisional partner in the electric field (mainly quadrupolar) of a hydrogen molecule but, for weakly polarizable species such as He, contributions due to electronic overlap at short distances are also important [45].

The absorption cross sections of H_2 are mainly induced by $\text{H}_2\text{-H}_2$ and $\text{H}_2\text{-He}$ collisions but on the Giant Planets and Titan other molecules can collide making this process possible.

According with one of the main code available [9] about this kind of absorption, coefficient for $\text{H}_2\text{-H}_2$ and $\text{H}_2\text{-He}$ interactions have been calculated for each atmospheric layer on our pressure-temperature grid and for each wavelength.

We mention that other studies [43], found different values for these coefficients, especially in the $5\ \mu\text{m}$ region, making this work strongly choices dependent.

Always in Figure 3.6, the absorption coefficient for $\text{H}_2\text{-H}_2$ and $\text{H}_2\text{-He}$ CIA is shown on bottom. Absorption of hydrogen and helium vary smoothly with wavelength, being the *continuum* level in Giant Planets atmospheres.

3.4.3 Transmittance of gases

Given the absorption coefficients of the various gases in the atmosphere, the emerging radiance for a real atmosphere may be calculated.

Since line strengths and line widths are function of temperature and pressure and since atmosphere are extremely inhomogeneous in both respects, the monochromatic transmittance at wavenumber ν of a path through an atmosphere is expressed by the (3.12):

$$\mathcal{T}_\nu = \exp \left[- \frac{1}{\cos \theta} \tau_\nu \right]$$

where

$$\tau_\nu = \int_{l_0}^{l_1} k_\nu^l(l) q(l) dl$$

Looking at this formula the optical depth seems to be a linear function respect with the abundance of a species. This is not completely true. When both self- and foreign-broadening became important in fact, monochromatic gaseous absorption coefficient computed for some mixing ratio profile cannot be used for different abundances.

This problem can be solved considering opacity computations for only some temperature, pressure and abundance profiles, and to repeat the entire computation for any other conditions. This is the approach we adopted in all the computations of synthetic spectra for data simulations.

In order to evaluate the depth of the sounding for understanding the theoretical atmospheric levels where the maximum signal comes from, we have calculated the Weighting Function and the Contribution Functions for all of the species and for the total atmosphere as well.

If we consider again the expression (3.14) for the radiance:

$$I_\nu = \varepsilon_\nu B_\nu(T_0) \mathcal{T}_{\nu,0} + \int_0^{\tau_0} B_\nu(T(z)) d\mathcal{T}_\nu(z)$$

this formula can be written in terms of altitude as well, being the transmittance and the optical depth quantities depending on the considered layer. The expression is:

$$I_\nu = \varepsilon_\nu B_\nu(T_0) \mathcal{T}_{\nu,0} + \int_{z_0}^{z_1} B_\nu(T(z)) \frac{d\mathcal{T}_\nu}{dz} dz \quad (3.17)$$

where we can define the other quantities:

$$\text{WF} = \frac{d\mathcal{T}_\nu}{dz}$$

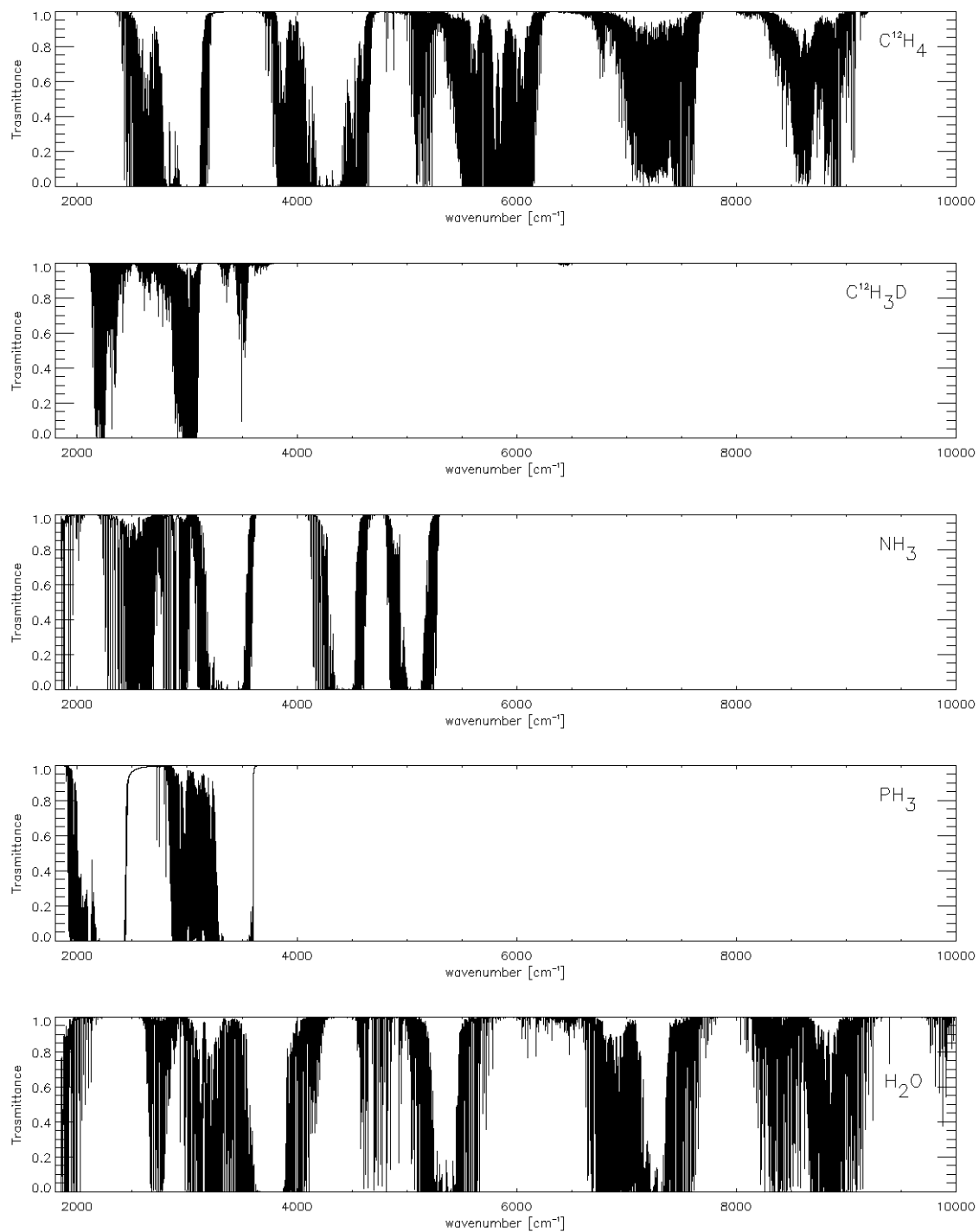


Figure 3.10: High resolution transmittance on monochromatic grid for $^{12}\text{CH}_4$, CH_3D , NH_3 , PH_3 and H_2O . All these quantities are calculated at 300 mbar and 94 k.

known as *Weighting Function* and

$$\text{CF} = B_\nu(T(z)) \text{WF} = B_\nu(T(z)) \frac{d\mathcal{T}_\nu}{dz}$$

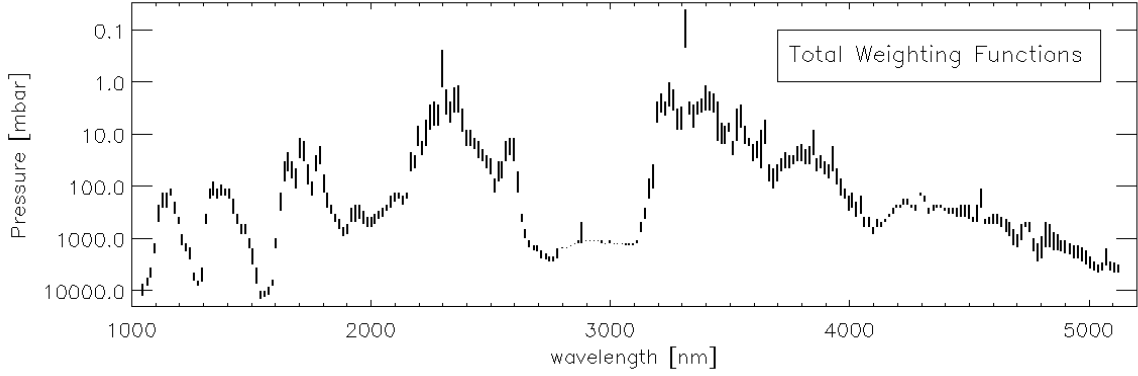


Figure 3.11: *Weighting Functions as a function of wavelength and pressure, as calculated by the model. The black bars indicate the pressure range where the signal comes from.*

known as *Contribution Function*, being the kernel of the radiative transfer integral. Being the WF multiply by Planck's function, the CF peak at greater pressures than those of the WF with a significant difference.

The WF are often used but this is suitable if the temperature gradient in the sounded part of the atmosphere is not too large [65]. The CF on the other hand, give more realistic pressure levels.

In Figure 3.11 we have plotted normalized Weighting Functions as functions of pressure for all the instrument channels. As can be seen in this figure, the pressure at which a weighting function peaks, and at which most of the measured reflected light will have been scattered, depends on the wavelength.

In the solar part of the spectrum however, it is not possible for the instrument to really sound that pressures, because the diffuse field due to scattering at lower wavelength. Even if the code gives one defined pressure level as peak level, we consider all the layers inside the 10% of the peak as real responsible of the signal at a specific wavelength. This is the reason of the vertical lines in the plots of Figure 3.11.

In Table 3.3 we summarize the main pressure levels for both WF and CF in some significative wavelengths in the thermal part.

VIMS channel [nm]	WF peak [mbar]	CF peak [mbar]
4500	229 - 432	827 - 1118
4570	433 - 544	1709 - 2262
4755	486 - 749	2774 - 3578
5041	3146 - 4528	4528 - 5787

Table 3.3: *Wavelengths and relative pressure levels sounded by Weighting and Contribution Functions for the thermal part. For every wavelength the pressure range of 10% of peak value is reported.*

In Figure 3.10, the molecules high resolution transmittance is shown.

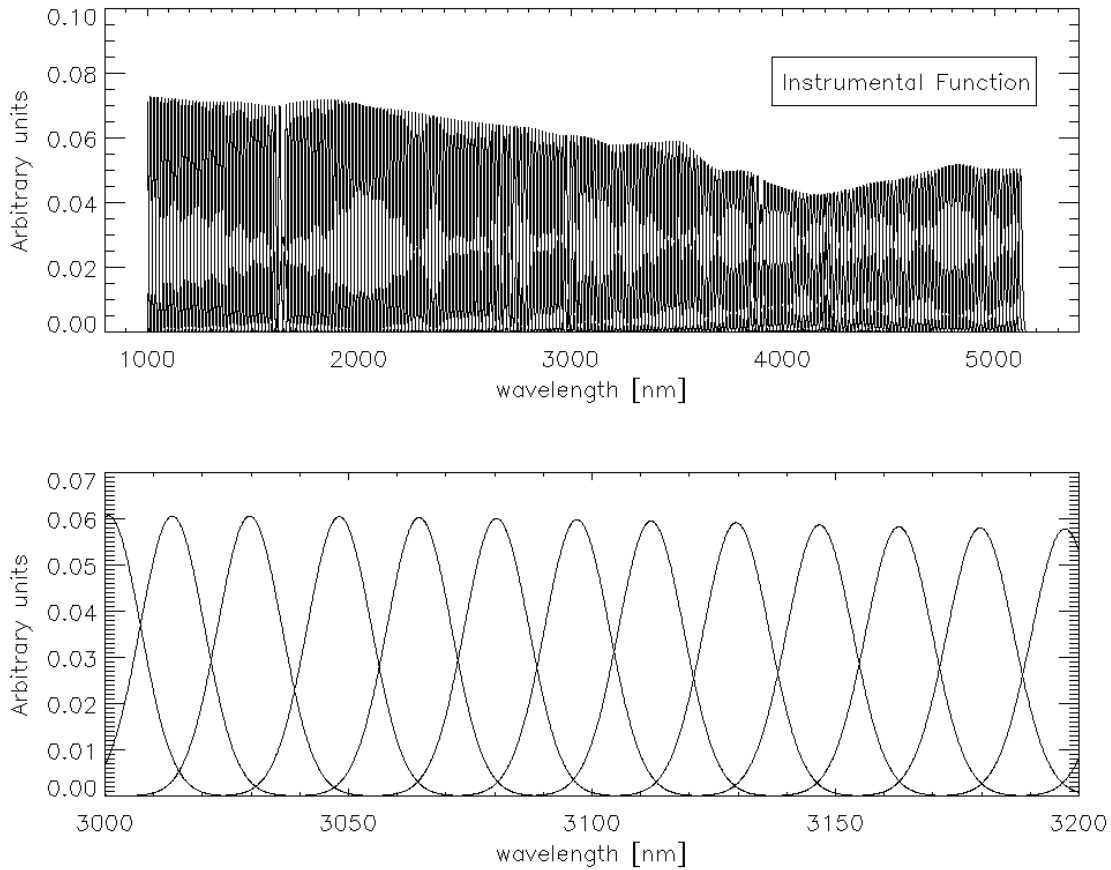


Figure 3.12: *Instrumental transfer function. For the convolution we use a gaussian with an FWHM taken from the header ancillary data. The resolution of the instrument decreases with wavelength. In the thermal region however seems to increase again. In the panel below, a zoom around 3.1 μm .*

3.4.4 Convoluted spectra

We said that the final step of the package **Arsm** was the convolution on the instrumental function.

The ARS code is designed to compute exact line-by-line calculations in wavenumber units. For each line of each gas, the absorption coefficient k_ν is calculated from spectroscopic parameters as line strengths and line shape, both of which are functions of temperature and pressure.

Since thousands of absorption lines may contribute to the absorption at a particular wavelength, it can easily be seen that such line-by-line calculations are computationally expensive and thus slow, although they are clearly the most accurate method available [10].

Having the instruments on board spacecrafts spectral resolutions lower than those available on ground base instruments, synthetic spectra calculations are compared with real measured spectra which very often do not need high resolution spectra to be

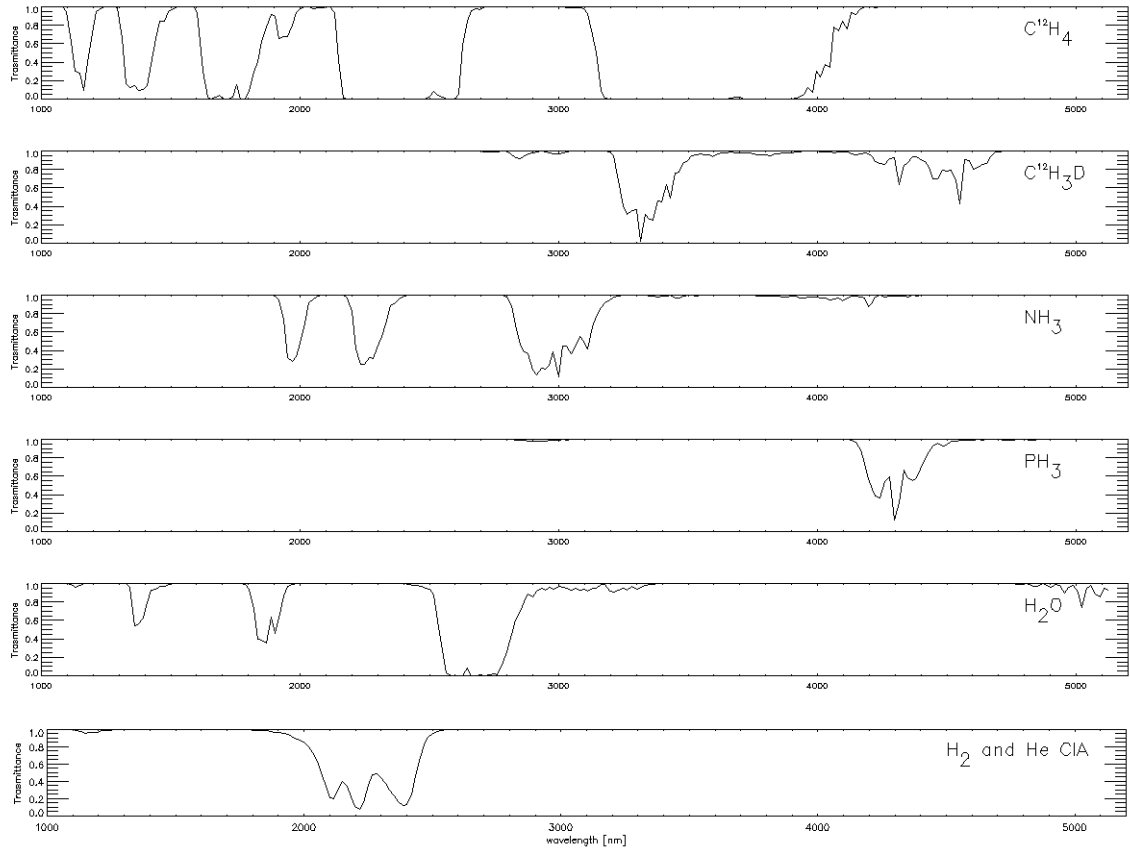


Figure 3.13: *Transmittance of the molecules involved in the model after the convolution at VIMS resolution. Quantities calculated at 300 mbar.*

compared with. We mention that alternative methods of simulation finite-resolution spectra exist and are much faster and slightly less accurate.

The *Band models* [7] and the *k-correlated* [13] are the most famous methods. In order to compare the simulated radiance spectra with the real ones, a convolution of line-by-line ARS outputs on the instrumental grid was needed.

The radiance, computed by ARS at high spectral resolution, has been convolved with a Gaussian function, gridded on the instrument's channel wavenumbers and then adapted to the wavelength units, in order to have the resulting spectrum in equally spaced wavelengths as the comparison with VIMS requires.

All the calculations have been done using the Full Width Half Maximum (FWHM) taken from the official ancillary data header file, linked to the observations. The instrumental transfer function in fact, shows how every channel FWHM is wavelength dependent as can be seen in Figure 3.12.

Figure 3.14, shows a typical example of monochromatic radiance convolved on the instrumental grid in the same manner previously described.

The red line can be consider as VIMS would see the high resolution spectrum. The convolution is the final radiance spectrum that will be compared with the real observation. The use of the same solar spectrum, official wavelengths and band centers,

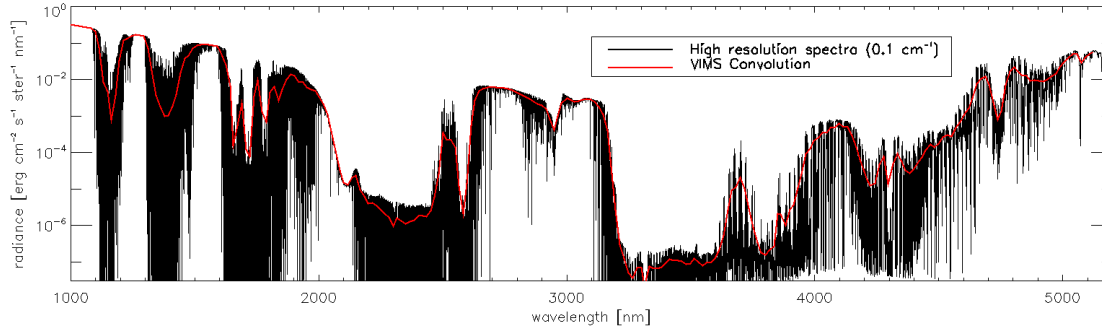


Figure 3.14: *Example of generic high resolution spectrum as generated by ARS line-by-line code, with all the specifications of our model. The red line is the convolution of the simulation on the instrumental grid, basically it is how VIMS would see the high resolution spectrum.*

radiance units and channel noise ensure the most similarity of the convolution spectra with the actual VIMS ones.

The same procedure is adopted for the monochromatic absorption coefficients and transmittances to compute the corresponding convoluted quantities. In Figure 3.13, the transmittance for every species calculated at 300 *mbar* and convoluted on the VIMS channels, are also shown.

3.5 Aerosols and clouds

With the exception of Uranus, all the Giant Planets radiate significantly more radiation than they receive from the Sun indicating a substantial source of internal heat. In the lower layers of the atmosphere air is heated from the interior. If the IR optical depth is high, then heat may not escape radiatively and instead the air rises convectively in order to transfer the heat upwards.

In parts of the atmosphere where the air contains volatiles, cooling caused by this upward motion of air parcels causes the condensation of cloud particles.

As material is transported upwards through the troposphere, temperatures drop and for some gases the partial pressure becomes equal to the saturated vapor pressure. Assuming the presence of cloud condensation nuclei, which appear abundant in the Giant Planet atmospheres, cloud layers may form and the gaseous abundance of the condensing molecules falls according to the saturated vapor pressure.

In the late 1960's the first quantitative models of the locations of condensate clouds based on thermochemical equilibrium theory were presented [52].

These models however are often complicated by uncertainties in the actual values of relative abundances [79].

The most abundant elements in solar composition which have the potential to combine with hydrogen to form clouds in the high troposphere are the oxygen (O), nitrogen (N) and sulfur (S). In addition to single condensate clouds, two-component clouds may also form in the atmosphere of the Giant Planet, of which the most important

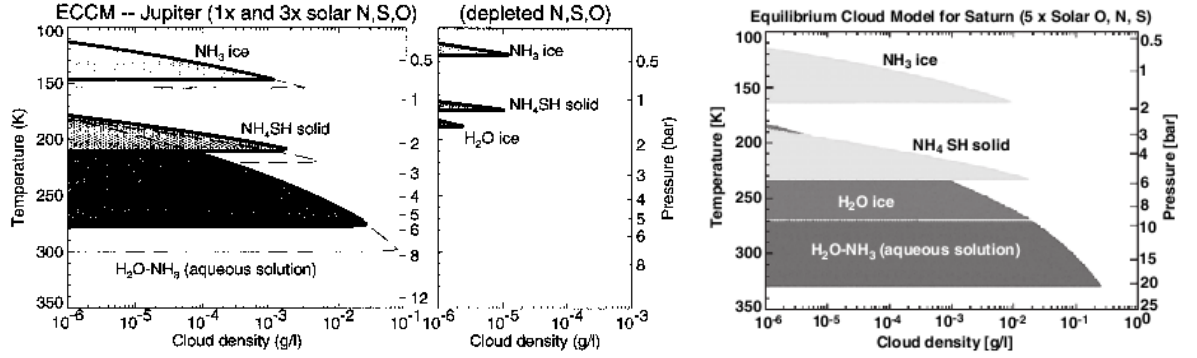


Figure 3.15: Cloud configurations for enhanced concentrations by a factor of five over solar composition for O, N and S for both Jupiter (left) and Saturn. The vertical location has been calculated by ECCM model [81].

is probably ammonium hydrosulfide (NH_4SH) in solid phase which may form by the reaction:



Even if this reaction depends on the relative mixing ratio of the initial components, both NH_3 and H_2S could be entirely depleted in the upper troposphere by this process. If the reaction is such that H_2S is more depleted than NH_3 , the remaining ammonia is available to form an ammonia ice cloud at higher altitude where the temperatures are cold enough to severely deplete this gas.

The cooler temperatures would saturate the ammonia in gaseous phase, forming haze particles in addition to the haze formed from upward eddy diffusion [61].

Radiative transfer modeling in the visible wavelengths allows to retrieve the upper cloud structure and the long-standing presumption has always been that the visible clouds of the two premier Giant Planets are made of solid ammonia particles.

According to the most recent theoretical thermochemical modeling [81], the Saturn's upper atmosphere is expected to contain three main cloud layers:

- An ammonia (NH_3) ice crystal layer centered at near $1 \div 1.5 \text{ bar}$
- An ammonium hydrosulfide layer (NH_4SH) centered at near $3 \div 4 \text{ bar}$
- A water layer centered at $8 \div 10 \text{ bar}$

The actual locations are uncertain because of the unknown abundances of the condensing constituents. Examined cloud microphysics however predict that the ammonia and ammonium hydrosulfide decks on Saturn are relatively thin, only lightly precipitating, and thus the equivalent of cirrus clouds on Earth [24].

Above the ammonia cloud however, thick hazes extend up to few *mbar*.

Through the process of convection, the NH_3 particles in the main cloud would be transported upward to fill in an extended hazy region throughout the middle and upper troposphere.

A strongly scattering haze is confined to the higher altitudes of the atmosphere as

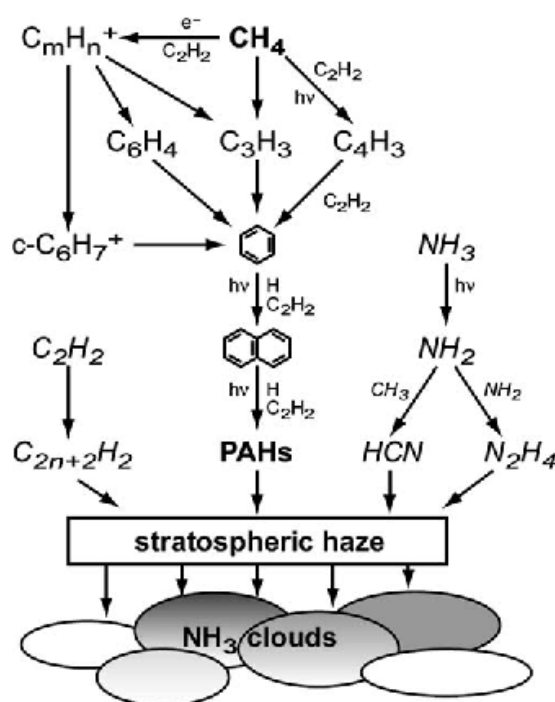


Figure 3.16: *Hydrocarbons production by photolysis scheme. Two types of hydrocarbons might be produced, a linear chain shown as the polymerization of acetylene and ring molecules starting with benzene [81].*

well and is mostly responsible for obscuring the activity occurring at depth, hiding Saturn's deep atmosphere.

In the stratosphere the aerosols formation is driven by photolysis processes.

Methane (CH_4) is a significant minor constituent of the stratosphere of Saturn. Photolysis of methane by solar radiation yields various product hydrocarbons of which the most abundant are ethane (C_2H_6) and acetylene (C_2H_2) [71]. Neither of these molecules however should exist under thermochemical equilibrium.

Models of methane photochemistry show a coupling between ethane and acetylene leading to more complex polycyclic aromatic hydrocarbons (PAHs).

The increase of temperature with height in the stratosphere implies the presence of additional energy sources. These sources include absorption of ultraviolet radiation from the Sun via gaseous photodissociation reactions and by stratospheric aerosols. Thus the temperature structure in the stratosphere depends critically on the vertical distribution of photochemical products in the same way that the stratospheric temperature profile of the Earth depends critically on the abundance of another photochemical product; the *Ozone* (O_3) [10].

At deeper levels, the water cloud is more massive and is more likely to be convective and sporadic with small areal coverage.

Studies based on cumulus parameterization show that water-based moist convection would occur on the giant planets and create a stable layer over a depth of about a scale height above the water condensation level [22]. This putative stable layer is too

deep to have been observed but is crucial to many shallow weather layer theories of Giant Planet circulations.

Anyway, the atmospheres of the Giant Planets contain various types of aerosol and cloud particles whose optical properties and vertical distributions vary across the planet and in time.

Knowledge of the particles spatial distribution and microphysical properties, such as their size, shape, and chemical composition, is important for understanding the atmosphere's chemical composition, its radiation field, and its dynamical processes. However, the clouds and hazes are not simply passive objects, but they also force atmospheric motions.

This is accomplished by heating and cooling the atmosphere at different levels, through the absorption or reflection of both sunlight and the thermal emission coming from the deep interior.

Clouds and aerosols play a role in the radiative and latent-heat terms of the energy budget, but the way in which an atmosphere reacts to such processes is still uncertain even for our planet [85].

To understand their radiative role in planetary atmospheres however, informations on particle optical properties and on their spatial distribution are for certain requested.

3.5.1 Aerosols optical properties

The determination of the physical and optical properties of cloud and haze particles in the stratospheres, upper tropospheres and deeper levels of the Giant Planets is essential for a host of atmospheric investigations.

In cloudy or optically thick aerosol regions, if the aerosol is located high in the atmosphere, absorption by the overlying gas is reduced and scattering from near the aerosol top takes place.

The main minor constituents of Saturn atmosphere is methane (CH_4). In the upper part of the atmosphere, solar photons photolyze this gas and the primary products of these chemical interactions evolve to heavier organic compounds that are likely to associate into the particles of haze layers that cover the planet.

The different theories and models that have been put forward to explain the characteristics and properties of the haze composites and the other clouds require a knowledge of their optical properties, which are determined by the complex refractive index.

The absorption of the radiation field propagating across a medium in fact, is directly proportional to the imaginary part of its refractive index at the considered wavenumber.

In our model we consider always spherical particles although, as pointed out by different authors [67], particles in Saturn atmosphere are expected to be irregular. Even if particles in Saturn's atmosphere are not simple spherical, however there is not a numerical code that can reproduce the single scattering properties for the broad range of particle shapes and sizes expected to find in the atmosphere of Saturn.

Aerosol particle sizes are not identical and a monodisperse distribution cannot represent the actual cloud composition. On the other hand, their radii can be represented by many different functions, such as *power-law function*, the *modified gamma distri-*

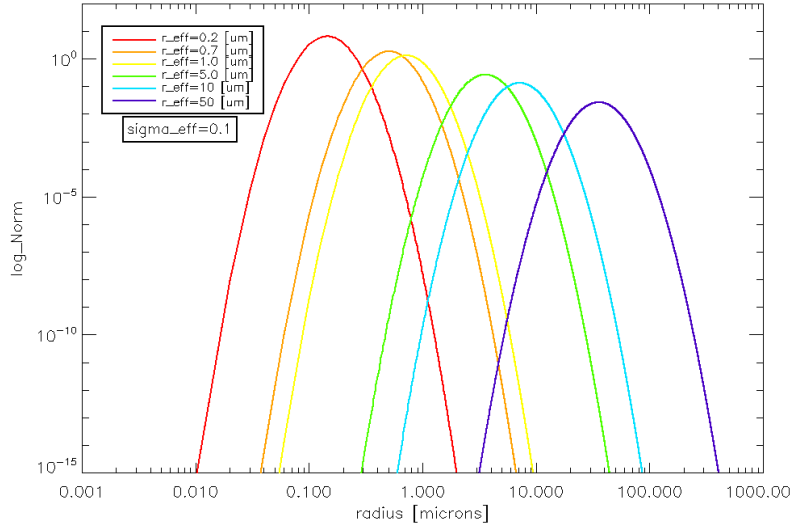


Figure 3.17: Log-normal size distribution for different particle radii. For the spread of the radii a constant value of 0.1 has been adopted.

bution function, and the lognormal distribution function [11].

We use this last option to vary the radii dispersion of our aerosol model.

Letting $n_d(r) dr$ be the number of particles per unit volume in the size range between r to $r + dr$, the aerosols are distributed in size according to a lognormal size-distribution as follows:

$$n_d(r) \propto \frac{1}{r} \exp \left[-\frac{1}{2} \left(\frac{\ln(r/r_m)}{\ln \sigma_m} \right)^2 \right] \quad (3.19)$$

where r_m is the modal radius and σ_m is the width of the distribution.

To limit the number of free parameters, we have set σ_{eff} to 0.1 that gives a value of $\sigma_m \sim 1.36$. This value makes the size distribution broad enough to avoid resonance effects without making the distribution extremely wide. The use of a different value of sigma has a slight influence on the final results without changing the general aim of this work, so we fix the value of $\sigma_{\text{eff}} = 0.1$ in all the calculations.

Figure 3.17 shows the distribution for different size of the particles.

In order to model the upper stratospheric haze, several microphysics models have been developed by different teams to simulate Saturn's aerosols nature but the explanation of all the evolution of the path from the methane photolysis to macromolecules and then to aerosol particles is not yet well understood.

Often the models fix the value of the real part of the refractive index which corresponds to the value for the expected condensates in Saturn's stratosphere [36].

The interpretation of a variety of atmospheric remote-sensing data also requires knowledge of the optical properties of the aerosols, which can be described in terms of the complex refractive index, to compute good reference models [30].

As a starting point for the refractive indexes of the spherical icy particles of the clouds, we have taken the results obtained by previous studies for the three different cloud layers.

The direct characterization of Saturn's aerosols is currently impossible; therefore, the experimental approach becomes the best way to understand the physical and chemical properties of the aerosols and to make progress in the interpretation of their role in upper atmosphere. In order to model the upper stratospheric haze we use a mixture of molecular nitrogen N_2 and methane CH_4 .

This kind of aerosols are expected to be in the Titan's upper atmosphere and many studies performed the study under well controlled experimental conditions for the characterization of the complex refractive index of an analogue of Titan's aerosols.

These authors [27] determined the real part n and imaginary part k of the complex refractive index $m=n+ik$ of the mixture N_2 - CH_4 . These final n and k values are used by modelers who compute the properties of Titan's aerosols in trying to explain the atmospheric dynamics and surface characteristic [78].

Moreover, a similar methodology has been use for the modeling of hydrocarbons in the upper stratospheres of Uranus and Neptune as well [28]. We assume these value for the real and imaginary part of the complex refractive index in Mie calculations for the composition of the stratospheric haze.

We are well mindful about the fact the a mixture of N_2 - CH_4 is not present in the stratosphere of Saturn but here, as first order of approximation, we use these value of n and k only to simulate the refractive index of the first layer of scatterers, in this context used only as reflectors of sunlight, without any physical correlation in respect with the actual atmosphere.

In Figure 3.18 the plot of these quantities are shown as function of wavelength. For the N_2 - CH_4 mixture the average value of n is near 1.6. Other authors [70] give for the actual stratospheric haze of Saturn a value of n ranging between 1.43 and 1.55, making our assumption still valid in our approximation. Moreover, being aerosol optical properties generally wavelength dependent, we prefer to avoid a single refractive index value for every wavelength.

Specially designed experimental conditions provided by other studies [53] ranging from the far infrared to the near ultraviolet, give the optical properties for the simulation of the NH_3 ice cloud in our model.

Recent publications [32] are the source of the refractive index of the particles of the deeper cloud layer made of ammonium hydrosulfide (NH_4SH).

The optical constant of ammonium hydrosulfide ice and ammonia ice were obtained through transmission measurements of thin films using both a grating and a Fourier transform spectrometer.

In each layer we have taken into account we consider both absorption and scattering by aerosols and gas, in Figure 3.18 the plots of the real and imaginary part of the refractive indexes of all components used in this work are shown. The spherical shape of the particles is one of the assumption of our model only for model simplicity. Mie theory provides a very powerful tool for the calculation of optical quantities.

The merits of using radius r_{eff} as the independent variable of a size distribution depend on the application. In radiative transfer applications, r prevails in the literature probably because it is favored in electromagnetic and Mie theory.

There is, however, a growing recognition of the importance of aspherical particles in planetary atmospheres. Considering the low temperatures in the upper part of the atmosphere, especially in the upper troposphere, crystalline shapes instead of spheres

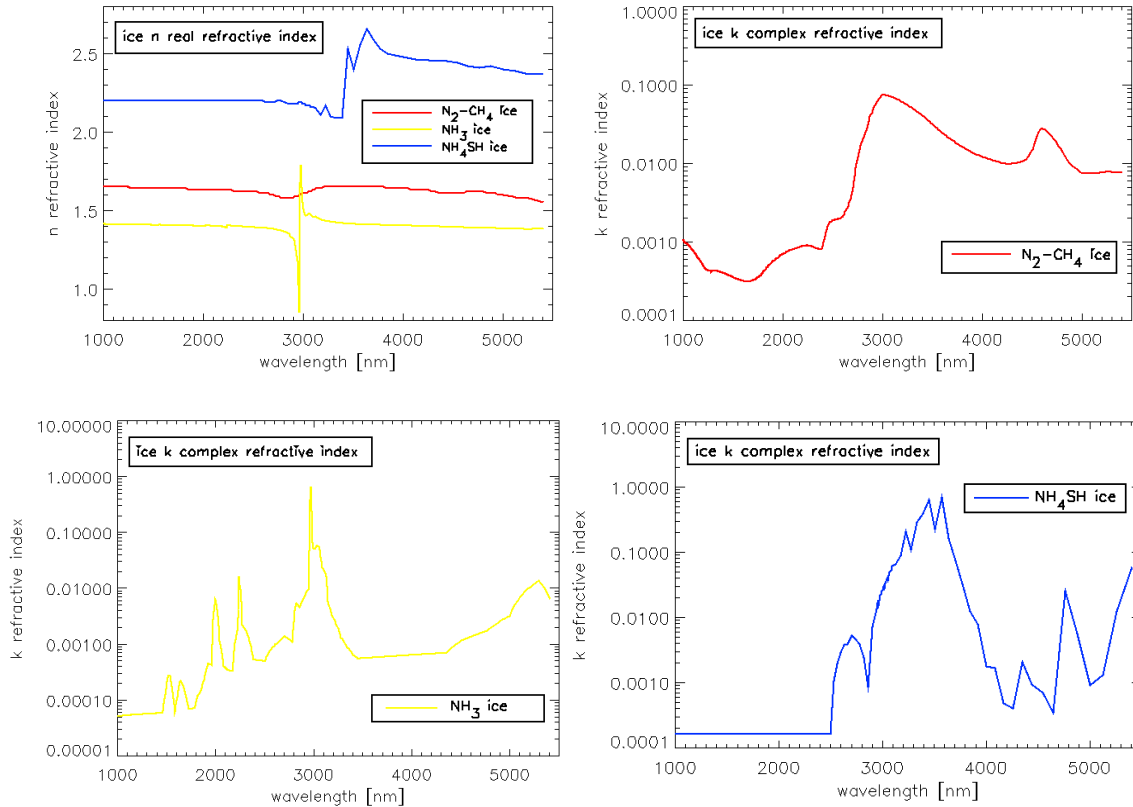


Figure 3.18: *Real and imaginary part of ices refractive index. On left (up) the real part is shown for all the ices. In the other plots the imaginary part is shown separately.*

are to be expected.

Fortunately the nonspherical nature of real ice crystals may often be ignored since a set of randomly orientated crystals is, to a first approximation, indistinguishable from a set of spheres with the same mean radius.

3.5.2 Clouds vertical profiles

The interpretation of observational data seems to indicate that a simple atmospheric model consisting of a reflecting cloud layer beneath an absorbing gas layer or a vertically homogeneous distribution of scatterers, cannot describe satisfactorily the observations [73].

Researchers inferred the aerosol distributions in the saturnian stratosphere and upper troposphere from observational results of ground-based telescopes, the *Voyager* space probes, and the Hubble Space Telescope (HST) assuming diffuse extended aerosol layers.

Some studies placed a sheet of infinitely opaque cloud of negligible thickness at the bottom of their model atmospheres. Other studies [50] adopted a more complicated cloud model similar to those for Jupiter and examined the opacities and altitudes of separated cloud layers.

The validity of these approach was later corroborated by the existence of separated cloud decks based on inversion analysis of near-infrared spectra of Saturn [34].

A three-layer model with a gas layer, haze layer and gas and a semi-infinite cloud deck to study the vertical structure of the giant storm erupted in the atmosphere of Saturn in September 1990 was adopted [51].

Other authors assumed a cloud structure with a continuous distribution of hazes with aerosols and gas uniformly mixed [67].

Some of the proposed structures include an aerosol free layer between the stratospheric and the upper tropospheric cloud. The reason for this structure was the impossibility of modeling the polarization measurements of *Pioneer 11* by assuming a single layer of scatterers [75].

All the results obtained suggest a cloud structure with two atmospheric regions (stratospheric haze and tropospheric haze) with relatively high scattering densities separated from each other by regions relatively free of scatterers [34]. This kind of structure was also successfully used in forward radiative calculations by other authors [50].

Taking into account the results obtained by all these authors we have assumed as starting point in our fitting algorithm an atmospheric distribution consisting of three atmospheric layers.

Starting from the top of the atmosphere our vertical structure is composed by:

- A stratospheric haze putatively made of crystals of $\text{N}_2\text{-CH}_4$.
- A tropospheric cloud of NH_3 ice.
- A deeper optically thick cloud of NH_4SH ice.

with aerosol-free layers between haze and clouds.

In order to model the initial number density of the particles, we use the simple equilibrium cloud condensation model (ECCM) as starting point.

The guiding principal of these models is that solid or liquid phase condensation occurs at altitudes above the altitude where the temperature and partial pressure thermodynamically favors condensation. The condensation levels of clouds then may be easily estimated from simple thermodynamics.

Considering a parcel of deep air that is lifted right up through the atmosphere without mixing with surrounding air, these kind of models can determine the general shape of the abundance profile of a condensable specie [10].

The ECCM predicts that if a parcel of air is raised up wards and the partial pressure of a gas exceeds the saturated vapor pressure, the exceeds is assumed to condense as cloud droplets and be lost from the parcel.

Following the ECCM, we have modeled the vertical profile of the clouds for the given value of mixing ratio of the condensable species.

In Figure 3.19 we show a schematic picture of a generic initial cloud positioning where cloud density expressed on the ordinate neglects sedimentation or vertical mixing or advection [81].

In our model the pressure level defining each cloud base layer is the pressure that in the final outputs indicates the position of the whole cloud in the atmospheric vertical profile. As said before, the pressure of the cloud base is one of the free parameters,

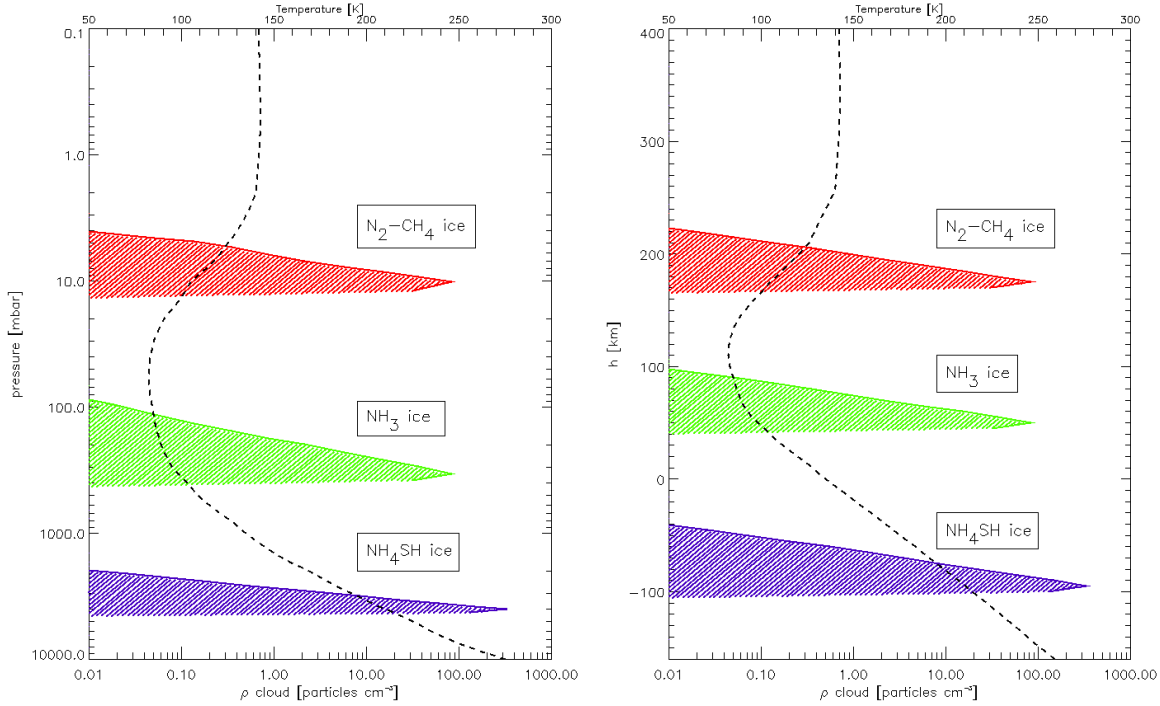


Figure 3.19: The two figures show schematically the vertical structure of Saturn's atmosphere according to our model. The ordinate variable is expressed in terms of pressure and altitude on left and right respectively. The p - T profile is also shown in dashed line with the relative temperature scale in the upper axis above the plots.

for all three types of cloud.

While the cloud bases calculated by the ECCM are fairly reliable, the cloud densities are likely to greatly exceed the actual mass density of the condensed clouds since they impede the precipitation and thus the re-evaporation of condensed aerosols and also horizontal mixing with nearby dry air [10].

In order to find a good fit from the generic initial cloud structure derived from the ECCM in fact, we also need to change the last free parameter, the number density of the particles.

The value of this last variable, is directly related to the size of the particles through the cross section and then to the total opacity of the cloud. So for the atmospheric structure different optical depths are also allowed.

Finally, the final atmospheric structure that results in our model consists of a stratospheric haze, putatively made of $\text{N}_2\text{-CH}_4$ without any actual physical meaning in respect with the atmosphere of Saturn, a tropospheric cloud made of NH_3 ice and a deeper thick cloud made of NH_4SH ice.

All these three clouds layers are separated from each other and from the deeper atmosphere by layers that are free of aerosol.

The final structure of Figure 3.19, is a generic configuration where the clouds profiles are obtained using the ECCM. Once the number density profile was defined however, we tried also to model others cloud profiles in order to understand if different shapes

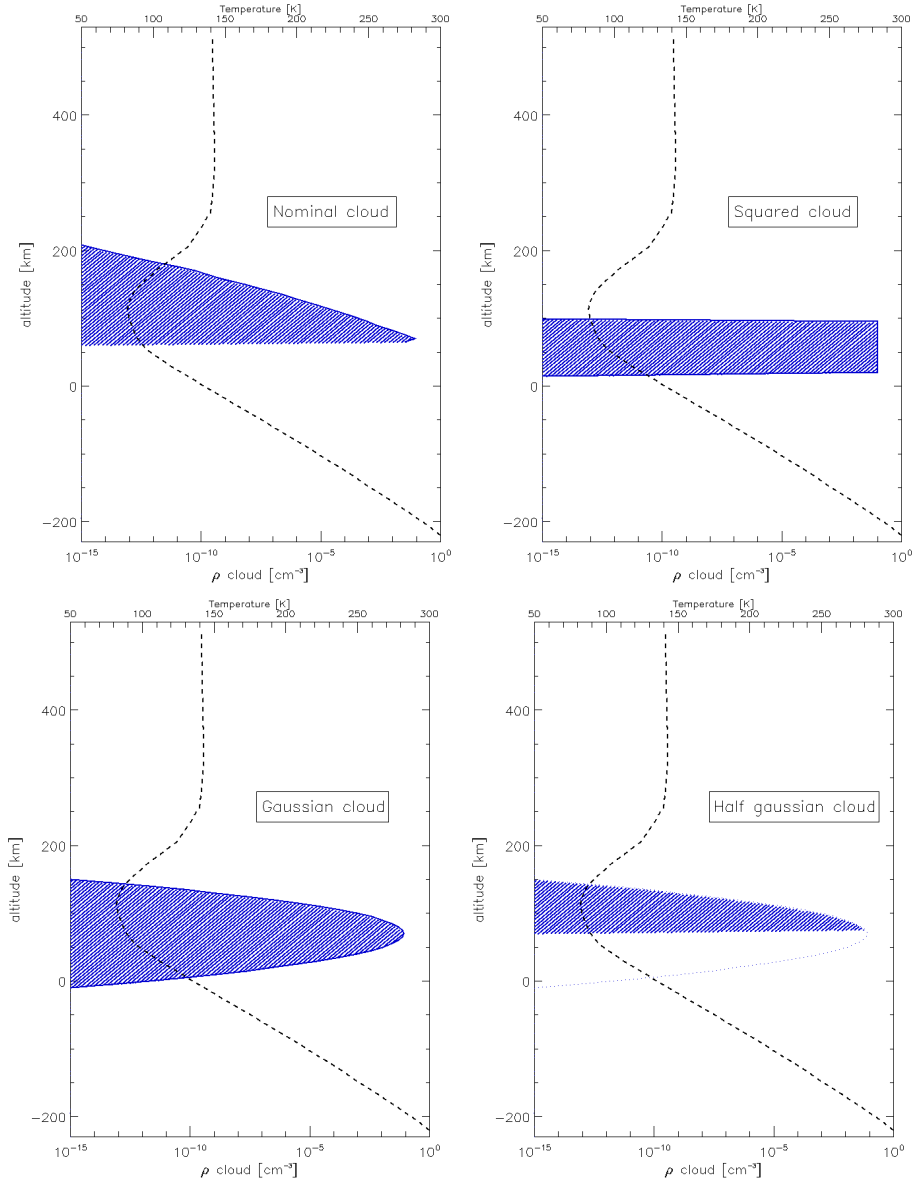


Figure 3.20: *Different cloud profiles used for model testing. The nominal profile (from ECCM) has been changed with other cloud shapes as squared, gaussian or half-gaussian. No significant differences in the final spectra were observed. The nominal shape has been adopted for all the simulations. In dashed line, the pressure-temperature profile is also shown.*

were able to reproduce a more realistic spectral behavior.

In the nominal cloud shape, the base of the cloud is the layer with the maximum number of particles, then the cloud number density decreases with altitude.

Considering the pressure of the layer with the maximum number of particles as the maximum of a gaussian, we have also modeled new shapes for the cloud profiles. Mainly we have considered three shapes of clouds: the *gaussian*, the *half gaussian* and the *squared* shape.

The results however, seem not to differ from the nominal shape, so we have decided to use the outputs of the ECCM.

3.6 The Radiative Transfer Model

The RTM is the final step.

Here, all the assumptions and calculations previously described, will be used.

The enrichment and/or depletion of the higher cloud as well as the deeper can be seen from the analysis of the spectra and from the images.

The expected vertical distributions and compositions of tropospheric clouds from thermochemical equilibrium theory and stratospheric haze from photochemistry, shows how different cloud layers are responsible for the observed spectrum of Saturn.

Because the solar part of the VIMS spectra is very sensitive to the aerosols vertical distribution in the upper troposphere and lower stratosphere, the effect of how different levels of aerosols and clouds affect the signal has been considered in the range between $1\ \mu m$ and $3.2\ \mu m$.

In the thermal range between $4.4\ \mu m$ and $5.2\ \mu m$, where the instruments sounds the deep atmospheric levels, the model reveals the need for thick deep clouds in order to fit the data.

In order to retrieve physical parameters from the comparison with the actual data of the observations, we have create a high resolution synthetic spectra databank in the range between $1\ \mu m$ and $5.2\ \mu m$, covering the whole instrument bandwidth.

For a given set of initial model free parameters we have calculated the synthetic radiance data for different observation geometry, comparing the results with the chosen observations at the same geometry.

3.6.1 The three clouds model

Modeling approaches with only one cloud layer cannot describe satisfactorily the spectral behavior in the range between $1\ \mu m$ and $5\ \mu m$.

Using Mie theory for spherical scatterers, it is found that small particles provide excellent near IR reflectors but are poor absorbers at $5\ \mu m$. On the other hand larger-sized particles are good $5\ \mu m$ absorbers but poor near IR reflectors.

Hence, simultaneously matching both the near IR and $5\ \mu m$ parts of the spectra requires minimum two cloud layers; a uniform cloud composed of small particles and another one of larger particles of variable optical depth well below, where they cannot interfere too much with the near IR reflectivity.

So in order to find the same spectral behavior in our model, we have tested it with a generic observation of VIMS at Saturn, using only one cloud layer, two cloud layers and three clouds layers, in order to compare the results.

In Figure 3.21 a generic observation of the South Pole of Saturn is shown. The image is taken at two different wavelengths, in the near IR (at $1.06\ \mu m$) on the left and at near $5\ \mu m$ on the right.

The content of the images and its physical meaning will be explained in the next chapters, what we want to show here however is the comparison of the acquired spectrum with different cloud configurations.

In the images is highlighted a red little square indicating the pixel chosen for the comparison. In the plots below, the Saturn spectrum in the instrument bandwidth in linear and logarithmic scale is shown with spectral signatures of the main elements.

We use an ammonia ice cloud for this first test, introducing after the stratospheric

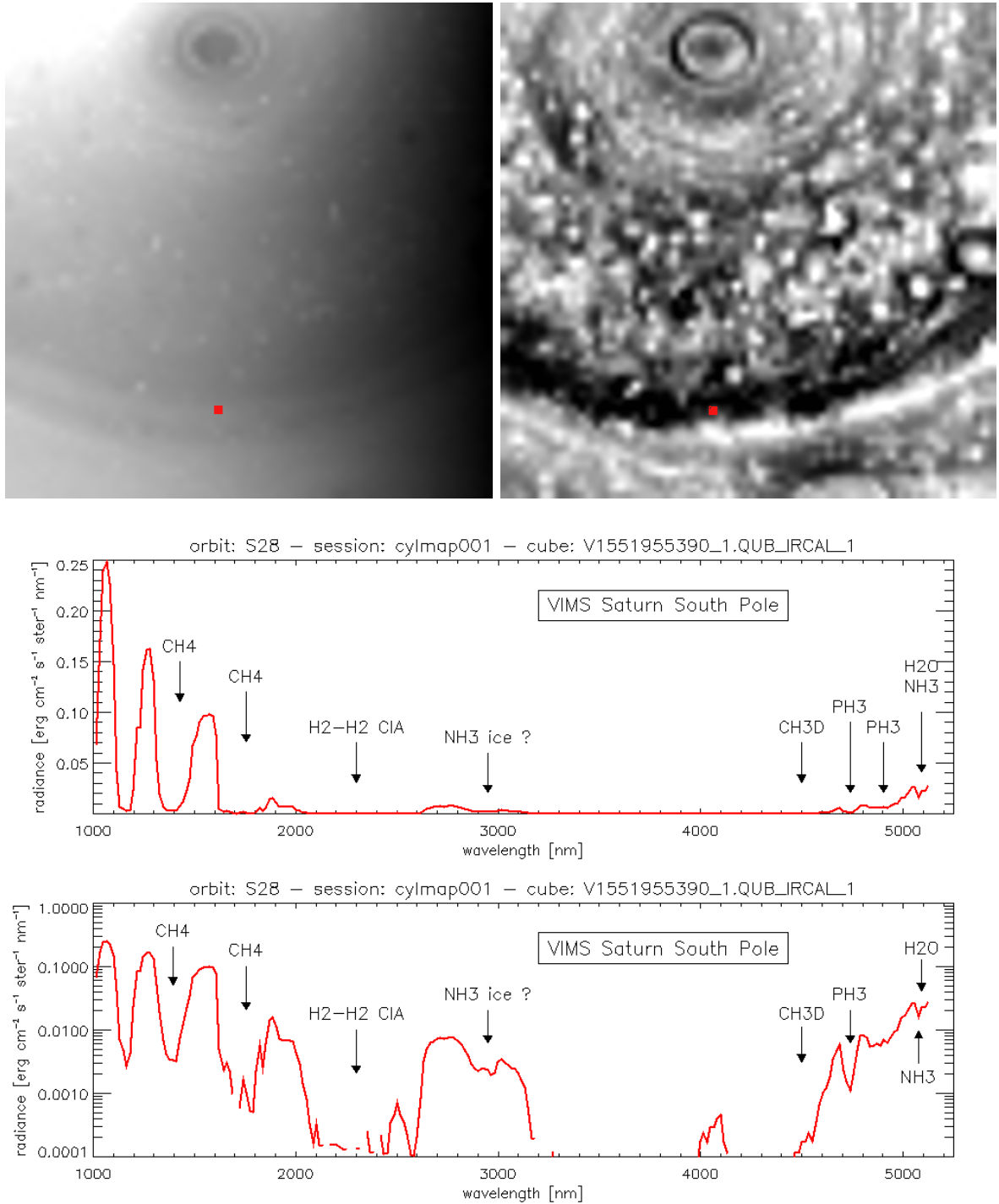


Figure 3.21: *Example of generic observation. South Pole of Saturn at near $1 \mu\text{m}$ (left) and $5 \mu\text{m}$. The red square indicates the chosen pixel and (below) the relative spectrum, in linear and logarithmic scale. Spectral signatures are also shown.*

haze and only in the end the deeper thick cloud.

In Figure 3.22 a unique cloud layer is responsible to take into account both the near IR and $5 \mu\text{m}$ part of the spectrum.

The discrepancy is evident.

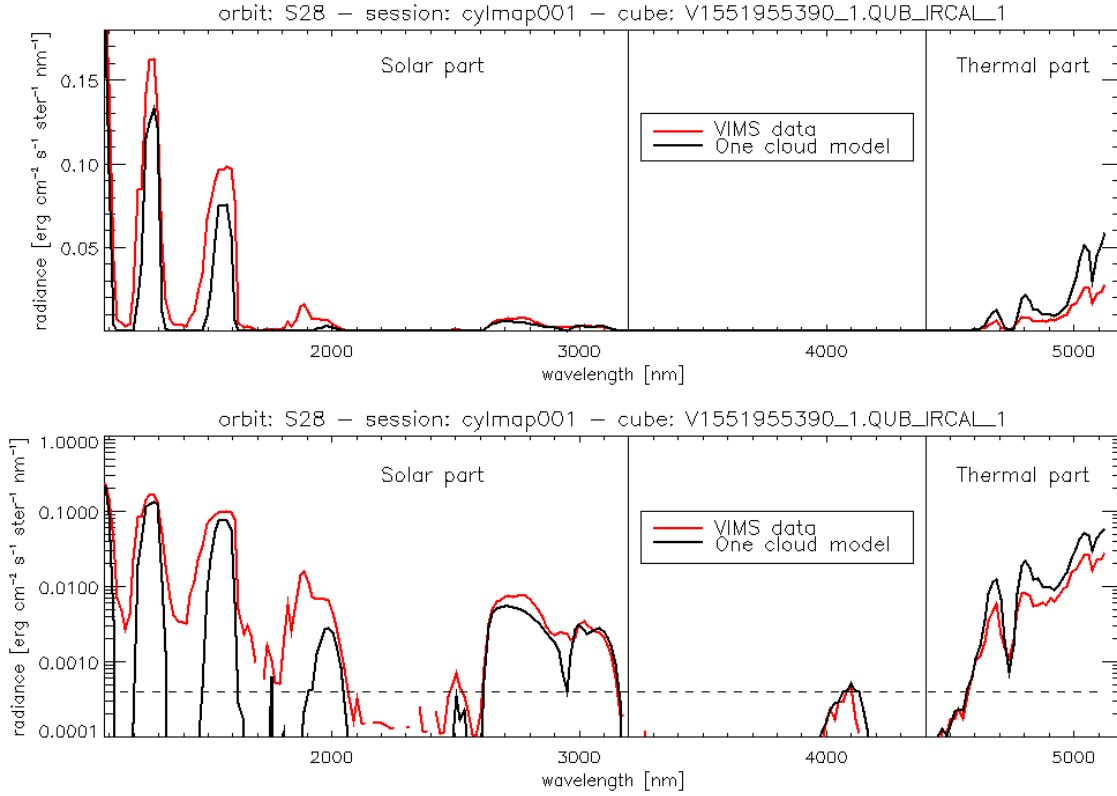


Figure 3.22: *One cloud model: this configuration is not able to reproduce the instrument signal. The fit is lost almost everywhere in the spectral range.*

The model spectrum represents the best configuration between the size of the particles, the pressure of the base of the cloud and the opacity of the cloud itself.

Neglecting by now the obtained values for the best configuration set of parameters, what we want to show is how the fit is completely lost. Hereafter the dashed line in all the plots represents the noise level. Below that level, the radiance signal used for the fit is not considered.

In the solar part⁷ the logarithmic scale shows well how the model cannot reproduce the bottom of the methane absorption bands.

The presence of scatterers at high altitudes is needed.

The fact that particles must be placed high in altitude comes from the total WF. Figure 3.11 shows how the wavelengths where methane absorption occurs (at near $1.15 \mu\text{m}$ and $1.4 \mu\text{m}$) sound the lower pressure levels (high altitude).

Huge differences with the observed spectrum can be seen even between $1.8 \mu\text{m}$ and $2 \mu\text{m}$.

In the thermal range between $4.4 \mu\text{m}$ and $5.2 \mu\text{m}$ the absence of an optically thick layer able to block the radiation coming from the deeper levels of the atmosphere is evident.

⁷Hereafter the term "solar part" is not related to any physical meaning of the electromagnetic spectrum wavelengths. It describes only the fact that at the near-IR wavelengths ($1.0 - 3.2 \mu\text{m}$) the sunlight is still spectrally active in that range.

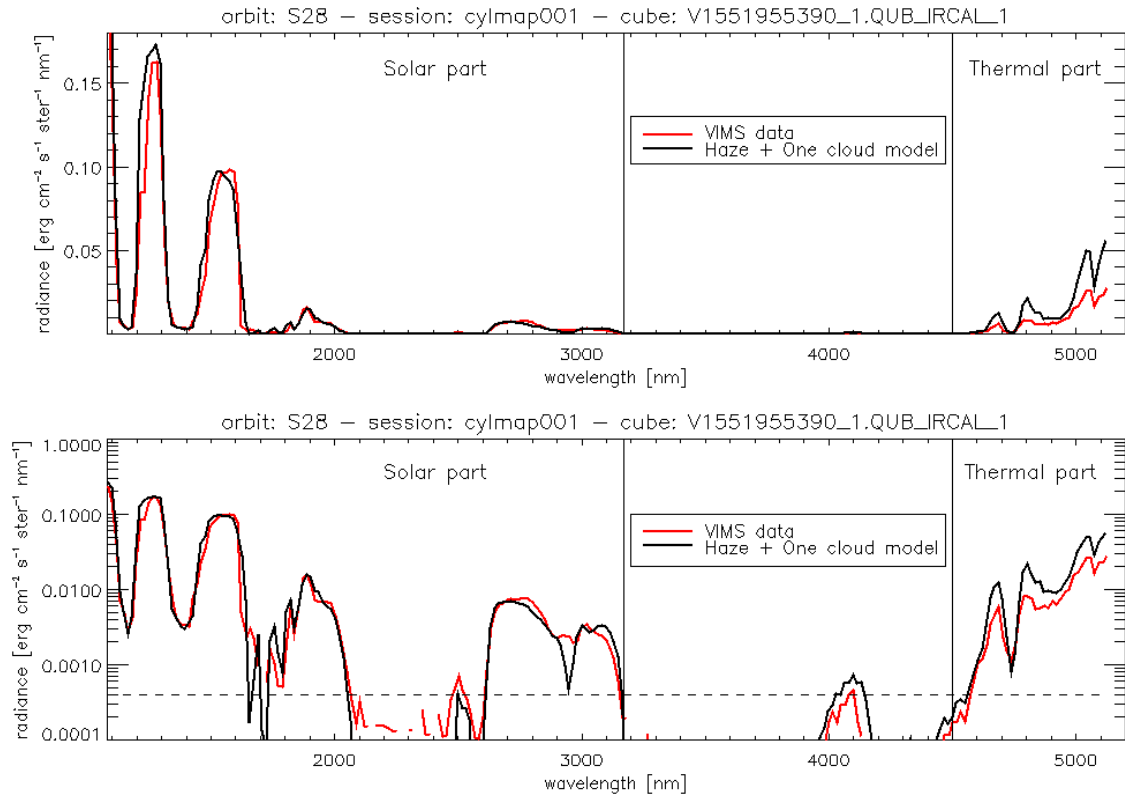


Figure 3.23: *Two cloud model: a stratospheric haze layer can reproduce the solar part but the fit is lost in thermal range.*

Being the cloud located near the pressures sounded by the near $3\ \mu\text{m}$ wavelengths range, the only part that seems to fit a little better is at that spectral range, with the only exception at $2.9\ \mu\text{m}$ where the ammonia fresh ice used in the model exhibits its strong absorption feature.

To verify the behavior of the model with the insertion of another cloud layer, we placed the stratospheric haze at higher altitude in order to find a best fit with the actual data.

Figure 3.23 shows the difference.

Now, the spectrum of the model is pretty acceptable in almost all the solar part.

Between near $1.6\ \mu\text{m}$ and $1.9\ \mu\text{m}$ the model is not able to fit the VIMS spectrum, this is true for all the simulations used in this work.

Nevertheless, the thermal part is still without any agreement and the need for a deeper cloud is more evident.

The game is now clear.

The cloud must be placed below the ammonia ice layer at higher pressure for the same reason explained before about the informations coming from the WF.

We included the optically thick cloud of solid ammonium hydrosulfide particles, that is expected to exist below the tropospheric cloud deck.

Figure 3.24 shows the final comparison.

Now we found a similar spectral behavior in all the instrument bandwidth.

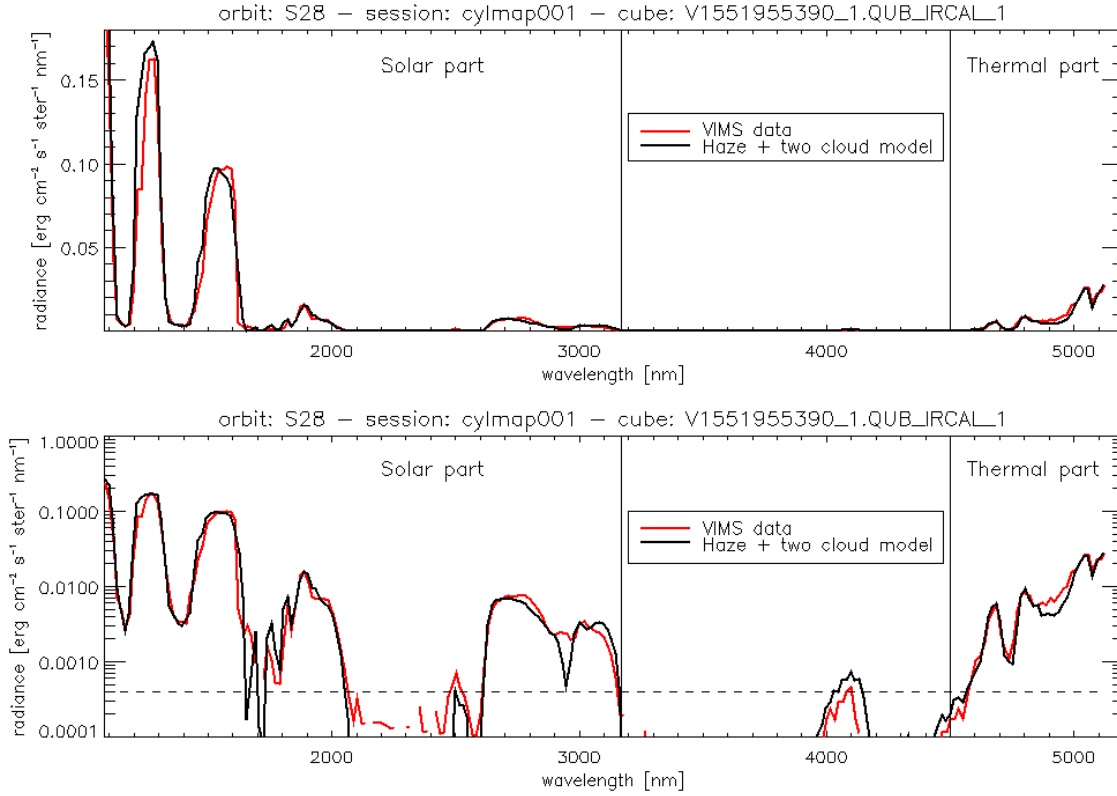


Figure 3.24: *Three clouds model: now, one haze layer in upper atmosphere, a tropospheric cloud and a thick cloud deck at deeper levels, are able to reach the instrument radiance level.*

The thermal range between $4.4 \mu m$ and $5.2 \mu m$ shows how the model is able to block the radiation coming from the inner part of the atmosphere of the planet and how the deeper cloud is important in order to reproduce the whole VIMS signal.

The fit is lost in the phosphine absorption band between $4.8 \mu m$ and $5 \mu m$. Here again this is true for all the simulations.

Looking at the three figure of the model we note that the solar and thermal part of our model are independent. When the stratospheric haze is placed in the one cloud model, the thermal part of the model remains the same.

The influence of the stratospheric cloud in the thermal range is negligible.

On the other hand, when the deeper cloud is placed in the two cloud structure, nothing happens to the solar part as request by our assumptions.

We remark that this is only an example to show the validity of the three clouds model and that the same VIMS spectrum used for the comparison represents only one of the possible actual atmospheric conditions.

3.6.2 The spectral databank

We said that for the analysis of VIMS spectra a spectral database has been created and used to find the best fit between the observed spectra and the synthetic ones.

For all the atmospheric layers in the thermal profile, we have considered as free parameters in the model the size of the particles of the clouds, the pressure of the base of the clouds in which they are distributed and the optical path⁸ of the clouds.

This last parameter is retrieved by a multiply factor for the number density of the particles. The multiply factor is the real free parameter being proportional to the optical path as shown in (2.68).

On the contrary, the fixed parameters for every layers are the pressure and the temperature, the absorption coefficient of the gaseous species, the chemical composition of the particles and their refractive indexes.

As initial value for the radius for stratospheric haze we have chosen a value of $0.08 \mu m$. This number has been varied up to $0.5 \mu m$ in steps of $0.02 \mu m$.

For the tropospheric cloud particles an initial value of $0.5 \mu m$ has been adopted, changing it between this value and $3 \mu m$ in steps of $0.05 \mu m$.

A previous analysis of the observed spectra behavior between $4.4 \mu m$ and $5.2 \mu m$ showed very flat absorption spectra in that range. So, for the deeper clouds scatterers a fixed value of $40 \mu m$ for the size particles of the deeper clouds has been chosen. This large particle size was chosen to ensure as flat an absorption spectrum as possible as required by the measures.

About the pressure levels of the clouds, the initial values for the stratospheric haze were fixed at $1 mbar$ and $5 mbar$, then a constant step of $1 mbar$ has been used until the $5 mbar$ level and, after that a constant step of $5 mbar$ until the final value of $100 mbar$.

For the tropospheric clouds, an initial value of $100 mbar$ has been adopted until the $1.5 bar$ level in steps of $50 mbar$.

For the deeper clouds, the pressure range is comprised between the $2 bar$ and the $6 bar$ level in steps of $0.5 bar$.

In order to minimize the number of free parameters in the model, we also checked the sensitivity of the model to these fixed values. We varied all free parameters by running the model in a loop sequence in which the parameters were varied from their minimum to their maximum allowed values. In this way we found the parameter range in which the model couldn't reach a good agreement with the observational radiance data.

So, we discarded all the combinations of parameters that were not able at all to reproduce the instrument signal.

Only those parameter combinations leading to a reasonable fit were investigated separately by a finer variation from the minimum to the maximum value in the new "good" values range.

This second step restricted the parameter solution space to an optimal combination of elements if compared to the requested computing time.

Nevertheless, due to the large amount of free parameters of our model we cannot consider our results as a unique solution. However, we have constrained the values of the input parameters of our model so that they would have a reasonable physical meaning.

Since the plane-parallel approximation produces erroneous results for small values of

⁸In this work the technical terms *optical path* can be found with the term *opacity*. In any case, the physical meaning is the same.

the cosines of the emission angles [4], only pixels with $\theta < 45^\circ$ are considered for the calculations reported in this thesis.

The illumination and emission angles however, are taken from the ancillary data of the observations and their values are used for the RT code.

As said before, the size particles, the pressure levels defining each cloud base layer and a multiply factor for the number density of the particles have been combined within the limits of sensitivity of our model.

The final output of our looping procedure, is a set of high resolution synthetic spectra describing different atmospheric configurations.

We remark that often a finer looping procedure is needed in order to find the best fit, considering the very different behavior of the actual data. Moreover, being completely independent by them, this database can be used for acquired observations and for future observations as well.

3.6.3 The fitting procedure

Once the databank spectra were available, a fitting procedure has been developed in order to find the final set of best parameters. This set defines an atmospheric structure which is the best representative of the actual spectrum.

From the total number of electrons per second stored in the detector, the noise for each channels can be expressed by [17]:

$$\delta R^{\text{VIMS}}(\lambda) = \sqrt{n_c [(n_\lambda + n_b)] t + n_r^2}$$

where n_c is the number of co-adds, n_r is the detector read noise and t is the integration time expressed in seconds.

Thus, for a generic single pixel spectra the radiance as a function of wavelength can be expressed as:

$$R^{\text{VIMS}}(\lambda) \pm \delta R^{\text{VIMS}}(\lambda)$$

However, in order to compare the simulation with the actual data, is not convenient to use single pixel spectra. This is due to the difference in the observed single spectra. Very often, it is better to consider an average of few pixels spectra for small areas.

The assumption that the averaged spectrum is representative of the whole area under observation is true until the radiance level of the pixels is almost the same, in order to avoid (when it is possible) an averaged signal coming from very different actual atmospheric conditions.

If so, for a generic set of N -pixels spectra we can consider for the radiance the expression of the *mean*:

$$\bar{R}^{\text{VIMS}}(\lambda) = \frac{1}{N} \sum_i R_i^{\text{VIMS}}(\lambda)$$

with $i = 0, 1, 2, \dots, N$ being N the number of the selected pixels spectra.

This quantity has two kind of uncertainties. Being the mean of different values, we can associate the *standard deviation* and the *standard deviation on the mean*, due to the instrumental noise.

These quantities are given respectively by:

$$\sigma^{\text{VIMS}}(\lambda) = \sqrt{\frac{1}{N-1} \sum_{i=1}^N [R_i^{\text{VIMS}}(\lambda) - \bar{R}^{\text{VIMS}}(\lambda)]^2}$$

$$\bar{\sigma}^{\text{VIMS}}(\lambda) = \frac{\sqrt{\delta R^{\text{VIMS}}(\lambda)}}{N}$$

The final error we associate with the VIMS radiance is $\Delta R^{\text{VIMS}}(\lambda)$ defined by:

$$\Delta R^{\text{VIMS}}(\lambda) = \max\{\sigma^{\text{VIMS}}(\lambda); \bar{\sigma}^{\text{VIMS}}(\lambda)\}$$

The fitting procedure is performed using $\bar{R}^{\text{VIMS}}(\lambda) \pm \Delta R^{\text{VIMS}}(\lambda)$ as input values.

Once the radiance of actual spectrum is so defined, the fitting procedure is carried out as follows.

The model begins to compare the value of radiance of the actual spectrum for every single channel with the value of radiance of the convoluted spectra in all the databank. We let the loop vary until a good fit with the observed data is obtained.

If we indicate the generic synthetic spectra of the databank as $R^{\text{ARS}}(\lambda)$, the quantity that defines the best match, is given by:

$$\chi = \sum_j \frac{[\bar{R}^{\text{VIMS}}(\lambda_j) - R^{\text{ARS}}(\lambda_j)]^2}{\Delta R^{\text{VIMS}}(\lambda_j)}$$

The final best fit is those which χ is minimum.

Subsequently, from the final synthetic spectrum we obtain the set of free parameters, representing the best final configuration of the atmospheric structure of our model. A well-known problem with this type of approach is that the discovered ‘hollow point’ of χ may be just one of the numerous local minima whose discovery process strongly depends on the initial sets of parameters.

A good setting of initial free parameters is essential to reach the correct global minimum. However, there was so little information available to make reasonable pre-suppositions about the global minimum that we had to cover as many initial settings as possible.

Due to this requirement, we integrated a grid-search algorithm into our code so that our initial parameter sets could systematically explore the vast parameter space within their physically reasonable ranges.

3.6.4 Final outputs

The final parameters are the size of the particles r_{eff} for every layer of clouds, the pressure of the base of the layers and the total opacity.

Neglecting any meaning to the Saturn actual cloud layers, we will often use the term *stratospheric haze* for the upper level nominally made of $\text{N}_2\text{-CH}_4$, *tropospheric cloud* for the NH_3 layer and *deep cloud* for the NH_4SH cloud deck.

The cloud base pressures and the size of the particles come directly from the best fit

parameters.

For the total opacity, we need to use again the expression (2.68):

$$\tau_\nu(z_b, z_t) = \int_{z_b}^{z_t} \sigma_{\nu,ext}(z) n_d(z) dz$$

where z_b and z_t are respectively the altitude of the bottom and the top of the cloud. The *extinction cross section* $\sigma_{\nu,ext}$ is related to the mean radius. The number density of the particles n_d defines the vertical cloud profile as a function of the altitude z and is obtained by a multiply factor that is one of the free parameter.

Assuming that in the parameter solution space the minimum value χ (which gives the best set of parameter) is close enough to its neighbour value $\tilde{\chi}$ so that we can consider a linear relation between the simulated radiance relative to χ and the radiance relative to $\tilde{\chi}$ and between the opacities obtained from both these quantities, the error of the opacity at one given wavelength can be estimated as follows.

For the given wavelength $\lambda_o = 5.1 \mu m$, we indicate the radiance at the best fit χ as $R_\chi^{ARS}(\lambda_o)$ and $R_{\tilde{\chi}}^{ARS}(\lambda_o)$ the radiance at $\tilde{\chi}$. For the opacity, the same expressions are: $\tau_\chi(\lambda_o)$ obtained from $R_\chi^{ARS}(\lambda_o)$ and $\tau_{\tilde{\chi}}(\lambda_o)$ obtained from $R_{\tilde{\chi}}^{ARS}(\lambda_o)$.

Considering now the absolute difference of these quantities:

$$\begin{aligned} \delta R^{ARS}(\lambda_o) &= \left| R_\chi^{ARS}(\lambda_o) - R_{\tilde{\chi}}^{ARS}(\lambda_o) \right| \\ \delta \tau(\lambda_o) &= \left| \tau_\chi(\lambda_o) - \tau_{\tilde{\chi}}(\lambda_o) \right| \end{aligned}$$

the error $\Delta \tau_\chi(\lambda_o)$ for the opacity of the best fit can be obtained considering the variation of opacity in respect with the radiance and assuming that the ratio of these quantities is less or equal at the ratio between the error of the opacity itself and the instrumental noise $\delta R^{ARS}(\lambda_o)$ previously defined.

In formulas we have:

$$\frac{\Delta \tau_\chi(\lambda_o)}{\Delta R^{VIMS}(\lambda_o)} \geq \frac{\delta \tau(\lambda_o)}{\delta R^{ARS}(\lambda_o)}$$

and the final expression of the error as:

$$\Delta \tau_\chi(\lambda_o) = \Delta R^{VIMS}(\lambda_o) \left| \frac{\delta \tau(\lambda_o)}{\delta R^{ARS}(\lambda_o)} \right|$$

so that the retrieved total opacity and its error can be written as:

$$\tau_\chi(\lambda_o) \pm \Delta \tau_\chi(\lambda_o)$$

this is the the expression for the retrieved value of opacity that appears in all the final tables of this thesis.

Finally, the final outputs of our code for every comparison between the VIMS spectra and ARS spectra are:

- r_{eff} - Size of the particles of the clouds.
- p_{cloud} - Pressure of the base of the clouds.
- τ_{cloud} - Optical path of the clouds.

We remark that all the opacity are referred at $5.1 \mu m$.

VIMS observations

The Cassini spacecraft is still sending home several gigabytes of data daily.

This mission has greatly improved our understanding of the Saturnian system and has returned many wonderful images.

The VIMS data are truly multi-disciplined, being related to atmospheric physics, retrieval theory, VIS and IR spectroscopy, meteorology, dynamics and many other fields of study.

The Cassini VIMS ability to probe to Saturn's atmosphere (and not only...) at all latitudes has opened up new prospectives for investigations.

In addition to continuing Cassini acquisitions, ground-based observations continue to improve in terms of both spatial and spectral resolution.

Moreover, the use of revised laboratory reference data should lead to a steadily improving understanding.

Understanding the Giant Planets in fact, is of interest not only in its own right but also in understanding how the entire Solar System and our own world in particular, came to be.

4.1 Data sessions

Living in its extended life, the spacecraft is orbiting in a polar trajectory giving us the possibility to see the poles as never before.

Originally discovered by Godfrey [33], the North Pole exhibits a weird and unusual hexagonal feature centered inside the region from near 76° to the pole¹.

The mechanism maintaining the hexagon is still poorly understood. Maybe due to *Rossby waves* dynamics, a perturbed zonal jet oscillates latitudinally in response to the restoring force of the latitudinally varying *Coriolis effect* [59].

At south, a complete different feature surrounds the pole.

VIMS images reveal a large, long-lived cyclonic vortex having a 4200 km diameter cloud free nearly circular region. This structure has features in common with terrestrial hurricanes and with other planetary polar vortices [84].

Comparison between the poles shows some similar feature and contrasts.

The first contrast is evident. The Hexagon.

¹All the latitude angles are expressed in planetocentric coordinates.

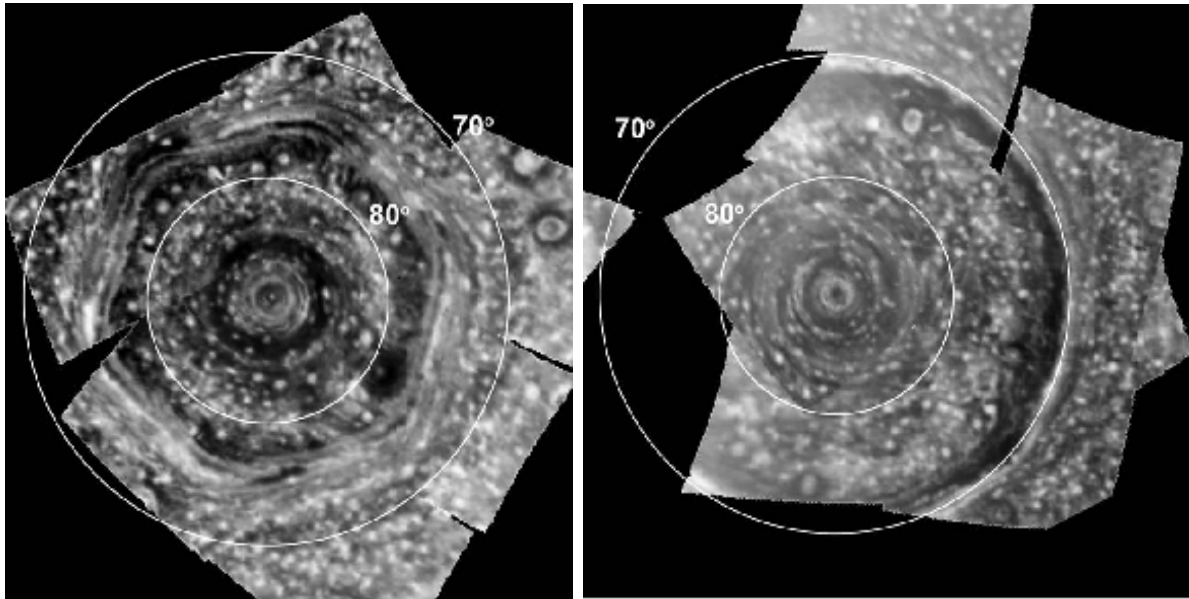


Figure 4.1: *On left, suggestive image of the dark and cold polar night of Saturn. The North Pole is shown with its weird creature: a perfect hexagon that reveals the real nature of Saturn's interior dynamics. On right the South Pole, with the vortex and its "eye" in the center. Both images are taken at near $5\ \mu\text{m}$ [59].*

Observing the Figure 4.1, it is clear that both poles show zonal structures with comparable number of discrete cloud features.

In the northern cyclone however, a discrete cloud feature is present but not in the southern where the center is more clear, akin to an eye of a hurricane.

Moreover, each of the poles has cloudy ring surrounding the center.

Now, Cassini is observing Saturn during its Northern Spring equinox started in august 2009 and there is great anticipation in how the return of sunlight to the North Pole region might affect The North Polar Hexagon (NPH) and warm North Polar Vortex (NPV) and how the loss of sunlight from the South Pole might affect the South Polar Vortex (SPV) [10].

One of the main aspect of the VIMS data is the great variability of the measured spectra both in visible and infrared channel.

If we consider the behavior of typical VIMS-IR spectra, the images reveal three major latitude regimes: the polar regions, the middle latitudes and the equatorial zone.

The spectra are strongly influenced by clouds and aerosols and reveal two major vertical regimes: the stratospheric zone above the interface with the troposphere near $100\ \text{mbar}$ and the troposphere itself.

The auroral processes drive the chemistry of the planet in the polar regions north of about 60° , here a stratospheric haze is optically thicker and darker than stratospheric haze at other latitudes.

At mid-latitude deep tropospheric clouds which probably form in free convection display substantial seasonal and nonseasonal variations. Distinct hazes layers at some latitudes are revealed by high spatial resolution limb images as well.

In this chapter, we will show the images used to test the model and verify the goodness of our choices.

The observational data used in this work consist of three images of Saturn taken in different orbits. In order to test the model we have studied images covering the South polar region, the South middle latitude and the Equatorial Zone.

Our goal is to test for the chosen spectra in each of these region, the validity of the model.

4.2 South Polar Region

VIMS high-resolution images reveal that in the center of the South Pole of Saturn, there's a warm cap where a large vortex surrounds the pole at latitude -87° [20].

The images show a *hot spot* in the center of the vortex. This hole is surrounded by a double cloud wall. Calling this structure the "eye" of the vortex, the eye has a nearly cloud free upper atmosphere above lower tropospheric clouds. Measurements from the projected shadows predict altitude differences in the eye wall of 40 km for the inner part and 70 km for the outer [84].

All around the cap until the thermal images reveal zonally oriented structures. Dozens of discrete cloud features visible in contrast to the thermal emission of the planet, dot this region.

A clear gap exists at that latitude in the cloud features. A relatively cloud free zone is visible near -70° in the right picture of Figure 4.1.

To test the model for the polar region, the observation we use is an acquisition of the South Pole ranging from near that latitude to the pole.

4.2.1 S28-cylmap001 session

The VIMS cube used for the south pole test is the V1551955390.1.qub taken during the cylmap001 session in the S28 orbit.

The acquisition was taken on march 2007 when the spacecraft was near 675.000 km from the planet. The spatial resolution for single pixel is 339 km , the solar illumination angle varies between 68° and 86° and the emission angle from 16° and 40° .

The Figure 4.2 shows the image at two different wavelengths: in the near infrared $1.06\text{ }\mu\text{m}$ and in the thermal one at $5.1\text{ }\mu\text{m}$. In the thermal image the latitude are also shown.

The image in the near infrared shows a very diffuse haze covering the region around the pole, it is possible however to see the change of regime near -74° where after that discrete cloud features look like bright areas, surrounding the pole.

In the thermal image, it is clear the differentiation of the structures.

The right picture in Figure 4.2 in fact, shows cloud structures located at different altitude, the image has been photometrically inverted showing the thermal glow of the emission of the planet in black and the silhouette of the clouds in white, where brightest features are relatively high in altitude. At $5.1\text{ }\mu\text{m}$ scattering by small aerosol particles is reduced and deeper cloud layers are easier to see.

This channel probes the deepest levels and shows how the opacity of the overlying stratospheric and tropospheric haze is revealed by its ability to block upwelling ther-

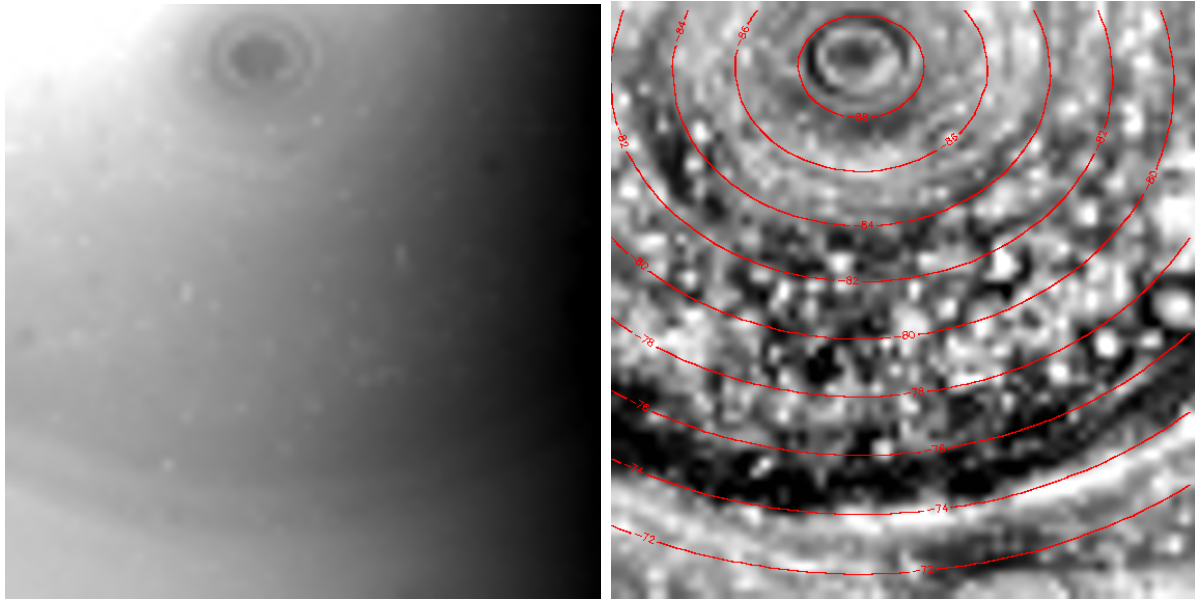


Figure 4.2: *Images of South Pole at solar and thermal wavelengths. On left the image is taken at $1.06\ \mu\text{m}$ and shows some bright cloud features. On right photometrically inverted image at $5.1\ \mu\text{m}$ where dozens of discrete cloud features are visible in contrast to the thermal emission of the planet. Latitudes are also shown.*

mal radiation. The signal of the black (and warm) cloud free track at -75° comes from the deeper levels of the atmosphere and the gray areas from the middle altitudes. The reason of the choice of this particular image is due to the need to have small emission angle in order to have an almost nadir viewing and to cover the edge of the polar region near -70° , here in the thermal part an evident cloudy "track" located at -73° is separated by a nearly cloud free zone at -75° .

The bottom of the thermal image is very interesting because three different atmospheric conditions are present.

A long bright cloudy feature is well visible at 73° latitude, indicating the top of a cloudy system of high opacity. Moving to the pole before the cloud free lane, there is a gray region parallel to the previous one, where a lower opacity is expected to be. After that, the hot lane mentioned before.

In Figure 4.3 the geometry of the observation is shown. To draw the isolines of the illumination and emission angle the data are taken from the SPICE² kernels.

4.3 South Middle Latitudes

At polar latitudes auroral processes might influence the stratospheric aerosol production but at midlatitudes, however, the stratospheric aerosol particles are expected to be of photochemical origin.

²Acronym of Spacecraft Planet Instrument C-matrix Events, is a tool for the interplanetary mission where all the geometry of observations of every single instrument in every single mission is stored in.

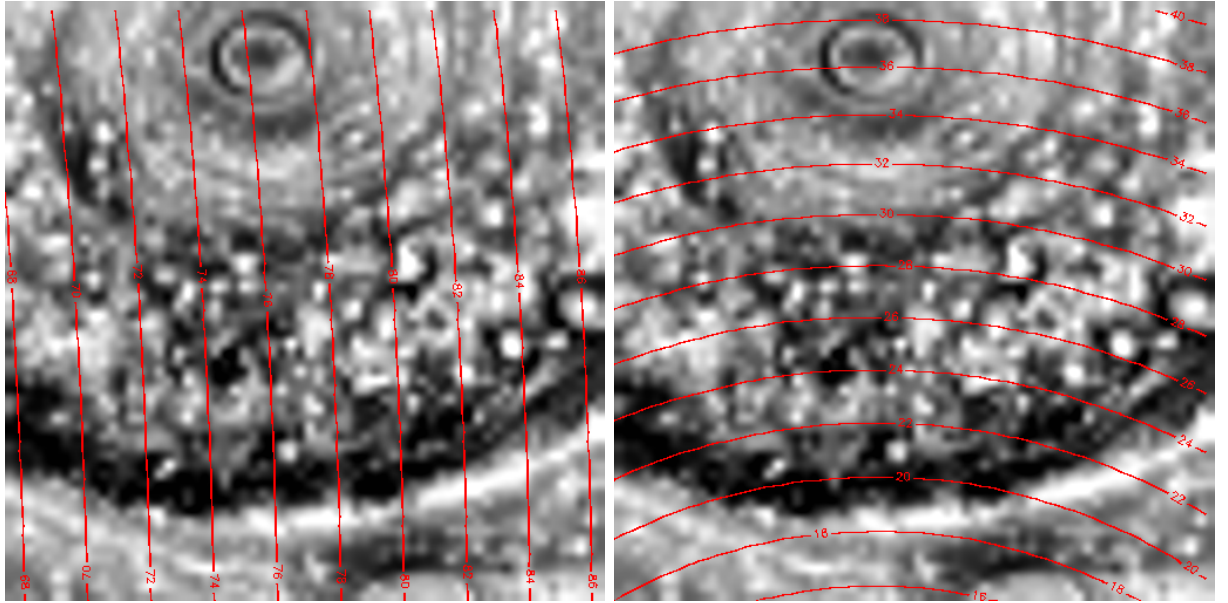


Figure 4.3: *Observation geometry: on left, isolines of the solar incident angle, on right of the emission angle (SPICE data).*

At different latitudes, both Saturn hemispheres exhibit a clear change in aerosols behavior. Looking at the VIMS images taken at midlatitudes this change is clearly shown. Between the midlatitudes near -60° and the south polar latitudes the aerosol optical thickness seems to attain a minimum value, which might indicate a boundary between different hazes [34].

The variations in the optical thickness however is different for the two hemispheres, the difference in the northern is more evident. This behavior was anticipated in previous studies [72]. Other studies have dealt with the hemispheric asymmetries in order to analyze this same phenomenon near -60° [70].

The Figure 4.4 shows the South Pole and the middle latitudes in two different ways. The panel above it is a RGB reconstruction and the panel below is in gray scale. Both images show the escaping thermal emission of the planet at $5.1 \mu\text{m}$ revealing deep cloud features. The near IR view in RGB exhibits the change in optical thickness mentioned before and the three main regimes are well visible.

The overlying haze reflects sunlight showing two changes: at 60° and equatorward of the cloudy band circling the planet near 75° south latitude. After, the thermal radiation dominates the third regime.

In order to verify the model, we use an image showing the first change at 60° .

4.3.1 S37-regpolmov001 session

The VIMS cube used for the south middle latitudes test is the V1581091877_1.qub taken during the regpolmov001 session of the S37 orbit.

The acquisition was taken on February 2008 when the spacecraft was at 800.000 km from the planet. The solar illumination angle varies between 60° and 90° and the

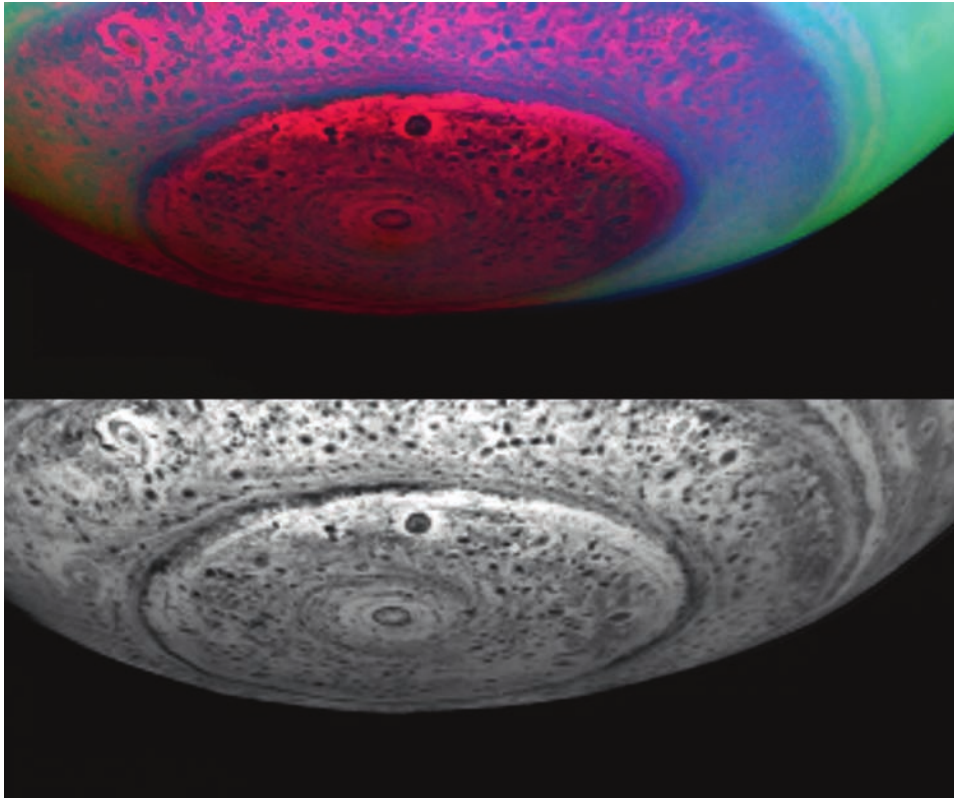


Figure 4.4: *Near infrared image of Saturn. The panel on top is an RGB ($R=5.1\ \mu m$, $G=4.1\ \mu m$, $B=3.1\ \mu m$) reconstruction showing three main regimes at different latitudes. The panel below shows the atmosphere illuminated from below, revealing deep cloud features in silhouette [58]*

emission angle between 30° and 75° .

Here again the figure (4.5) shows the image of the planet at the same wavelengths seen before, showing both the solar and thermal part.

In this case, the image in the near infrared shows the changing of the middle latitude. Before the -60° a diffuse sheet of haze covers the entire planet and after that is possible to see the top of cloud features disperse along iso-latitude lanes.

The bright region before the -60° shows the high optical thickness of the upper part of the atmosphere due to the stratospheric and tropospheric haze.

These haze layers located at different altitude, cover the deeper clouds visible in the $5.1\ \mu m$ image only.

The small-scale features visible at $1.06\ \mu m$ are brighter than the surrounding atmosphere and are probably the top of the high and relatively dense clouds composed of white ammonia ice.

The tropospheric clouds located at mid-latitude show a substantial seasonal and non-seasonal variation. Because their morphology these features resembles terrestrial cumulus and a freely convecting atmosphere is invoked to explain their formation hence often these clouds are called *convective clouds*.

However, the fact that other features are not visible in the methane absorption bands and appear bright in the visible and dark in the infrared seems to indicate that they

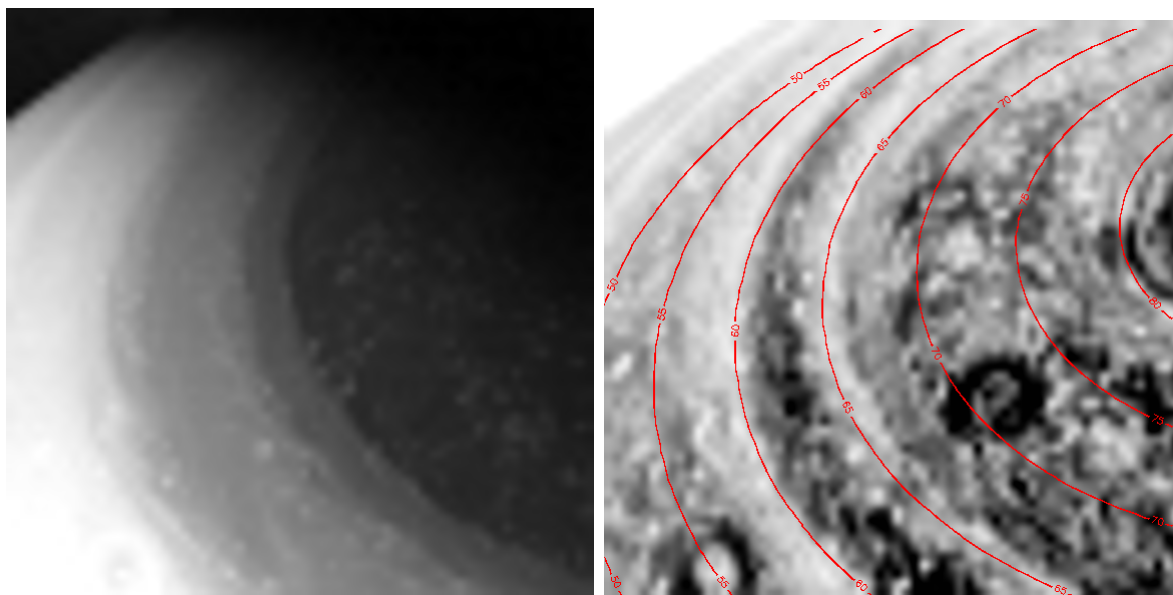


Figure 4.5: *Saturn's midlatitude images. Here again the planet is shown at $1.06\ \mu\text{m}$ (on left) and at $5.1\ \mu\text{m}$. At solar wavelength a diffuse haze covers the entire planet showing an evident change of regime near -60° . The top of discrete cloud features (probably white ammonia ice) are visible. The thermal image on right reveals two funny cloudy lanes at -60° and -65° separated by a relatively cloud free "hot" gap.*

are located in the deeper atmosphere, well below the 2 *bar* pressure level.

In the picture on the right in Figure 4.5, here again the image has been photometrically inverted showing the thermal glow of the emission of the planet in black and the silhouette of the clouds in white.

The new scenario now is different and reveals two distinct cloud lanes at -60° and -65° latitude. These two lanes of clouds are divided by a third lane relatively cloud free.

The oval near the lower-left corner of the thermal image, at nearly -55° is an *hot spot* region with a cloudy feature in the middle. Along the meridian to the pole, after the three lanes is visible another hot structure with a faint cloudy circle in the middle. This structure is located inside the third regime shown in Figure 4.4 where the thermal emission of the planet dominates.

In order to reproduce the visual effect of Figure 4.4, we have reproduced a RGB image using wavelengths of $1.26\ \mu\text{m}$ for blu, $1.49\ \mu\text{m}$ for green and $5.04\ \mu\text{m}$ for red.

Obviously, this false-color image is not what an human eye would see... but very often this kind of images result very useful because enhanced contrast brings out scientifically meaningful details. The result is shown in Figure 4.6.

Here, the change of the signal between the regimes is well visible.

From the equator until near -55° , the image shows a signal coming from the reflected sunlight by the upper haze, revealing a very uniform sheet that cover the planet at all the low latitudes.

A little bit before the -60° the regime change becoming darker well above (in alti-

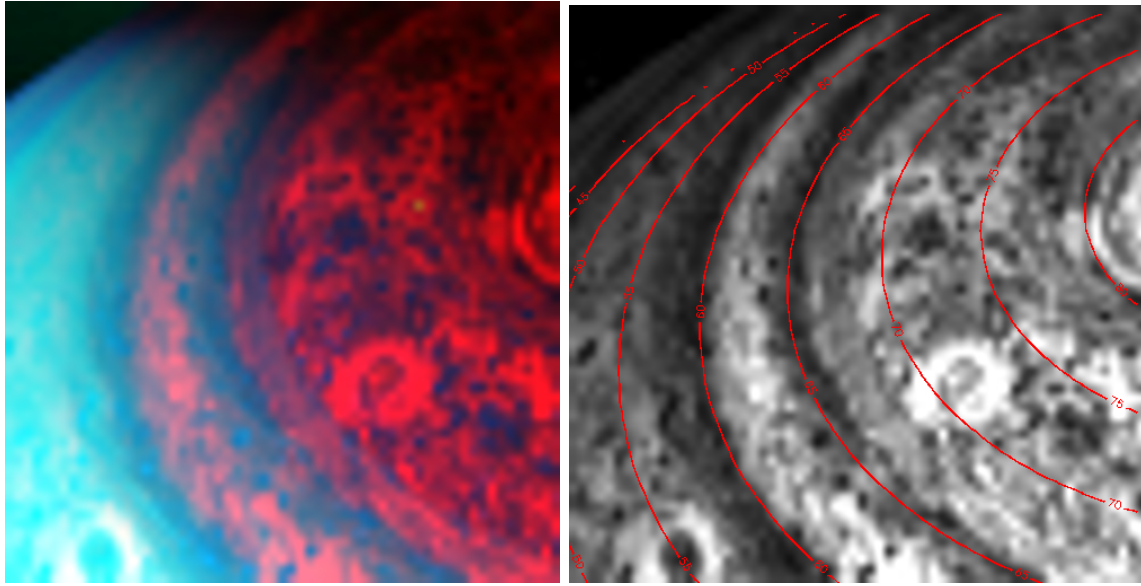


Figure 4.6: *False-colored RGB ($R=5.04\ \mu\text{m}$, $G=1.49\ \mu\text{m}$, $B=1.26\ \mu\text{m}$) image showing the regimes changing with latitude. On right, same image but in gray scale at $5.1\ \mu\text{m}$ not photometrically inverted.*

tude) the first lane of clouds.

At near -63° in the gap between the cloudy lanes, a faint red appears, revealing the escaping of thermal radiation in a relatively cloud free zone. Moving to the pole after the second cloudy lane where the signal become darker again, finally the red bright signal appears indicating the strong thermal emission of the planet.

The very different regimes can be recognized looking at the two *hot spot* structures mentioned before. The first near the lower-left corner of the image appears almost white and all the cloud free circle is still well visible, the second is in the thermal polar regime revealing the absolute absence of clouds.

Here again, in Figure 4.7 the geometry of the observation are shown.

4.4 Equatorial Zone

Modern observations of Saturn cover an entire seasonal cycle of the planet.

Both ground-based and spacecraft measurements during the past three decades show that Saturn has gone through a full seasonal cycle.

From those measurements clouds and haze are higher and thicker in the northern mid-latitudes relative to the southern hemisphere near the end of southern summer and shortly after equinox [67].

The opposite asymmetry has prevailed thus far into the Cassini mission in 2004.

The data indicate that the upper vertical structure consisting of a stratospheric haze layer and a more dense upper tropospheric haze layer were thinner and deeper in the north relative to the south.

Saturn's hemispheric asymmetry is changing, in expectation with observations taken

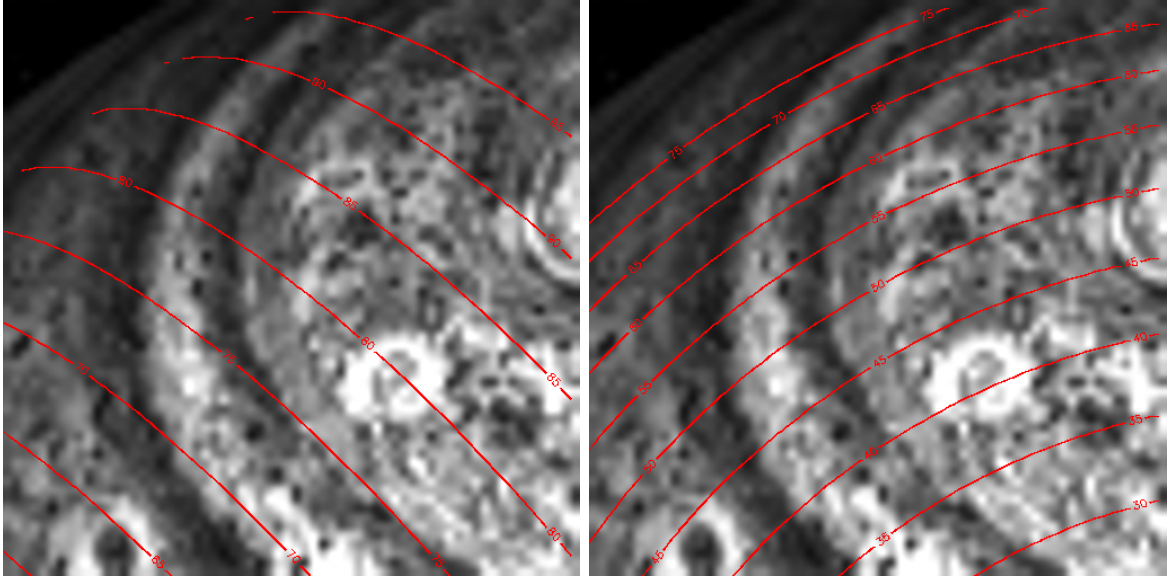


Figure 4.7: *Geometry of illumination and emission angle for the midlatitude observation (SPICE data).*

more than thirty years ago showing an asymmetry opposite to what was observed by Cassini instruments until 2008. Over the next year the asymmetry reversal is expected to be complete [12].

The asymmetry between North-South hemispheres however is broken by the tropical band (typically $\pm 10^\circ$) where the largest scattering densities in the upper tropospheric haze layer are found. The spatial distribution of particles appears to be very variable with latitude both in the stratosphere and troposphere.

The Equatorial Zone is consistently a region of higher and thicker clouds.

This is also a region which experiences occasional major cloud eruptions which have long-term influences on cloud opacity.

This is evident in the VIMS data where the radiance signal is high compared to the other latitude of the planet.

The equatorial region is the last atmospheric condition we use to test our model.

4.4.1 S18-globalmap002 session

The last VIMS data we use to test the model with the equatorial region is not a single cube but a three cubes mosaiking.

The cubes used are the V1519312329.1.qub for the northern part of the mosaiking, the V1519312751.1.qub for the equatorial and the V1519313173.1.qub for the southern part, all taken during the globalmap002 session of the S18 orbit.

The acquisition was taken on May 2006 when the Cassini was at 1.590.000 km from the target. The solar illumination angle varies between *solar zenith* (0°) and 55° for the southern hemisphere and 85° for the northern, the emission angle between 10° and 80° .

In Figure 4.8 three different images of Saturn are shown.

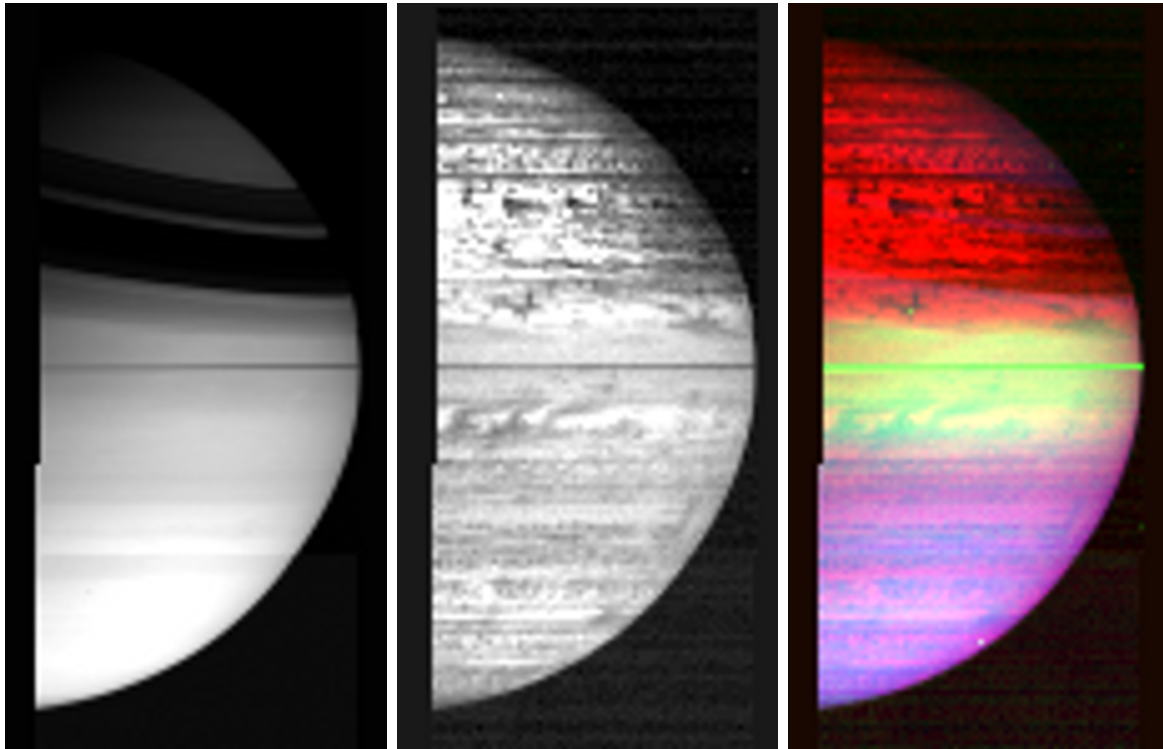


Figure 4.8: Entire planet mosaiking of three different observations. The panel on left shows Saturn at an atmospheric window ($1.06 \mu m$) revealing the different haze regimes with latitude. The black areas in the northern hemisphere are the projected Rings shadows. In the middle, same image but at $5.1 \mu m$. It shows the asymmetry northern-southern hemisphere and the uniform regime of the haze at Equatorial Zone. On right same previous wavelengths RGB image showing the reddish northern emission of the planet, the high scattering equatorial band and the reflected sunlight regime at southern. The faint line in the middle of every images are the Rings. Note the very low thickness compared to the main body.

The panel on the left shows Saturn at $1.06 \mu m$, in the middle at $5.1 \mu m$ and the right panel is an RGB taken at $1.26 \mu m$ for blu, $1.47 \mu m$ for green and $5.06 \mu m$ for red. The $1.26 \mu m$ image shows Saturn as a calm body where an haze covers the entire planet. It is possible however to distinguish in the southern hemisphere the same change in regimes seen in the previous closer acquisitions.

Several broad bands of hazes circle the planet, with little longitudinal variability and relatively little contrast between adjacent bands. Even if the channel used for this particular image should exclude any methane absorption, the image reveals qualitatively how cloud top altitude and optical thickness vary with latitude.

The darker areas in the northern hemisphere low latitudes are the Ring shadows projections and not atmospheric absorptions.

The $5.06 \mu m$ image in the middle shows clearly two main aspects of Saturn atmosphere: the asymmetry between northern and southern hemispheres and the total uniformity of the Equatorial Zone.

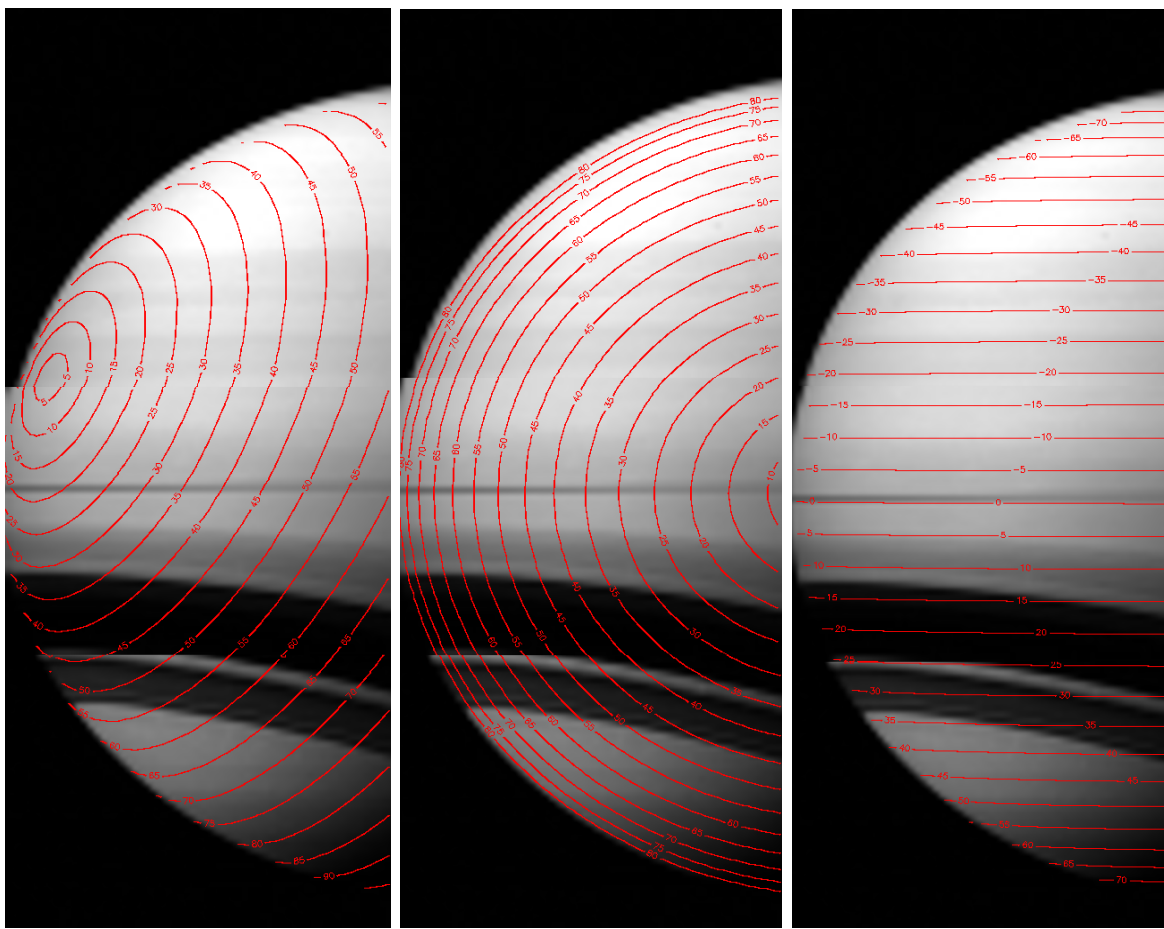


Figure 4.9: *Solar illumination, emission and latitude for the previous image (SPICE data). In the three panels, the planet is down-under (South is on top) in order to show correctly the values of geometry.*

This global view of the planet reveals how at the moment of the acquisition the overlying clouds were slightly thicker in the southern hemisphere as noted earlier about the asymmetry. Hundreds of small cloud features can be seen also. Moreover the northern hemisphere shows a series of cloud free zones more than in the southern. In contrast with the $1.26\ \mu\text{m}$ image, the thermal view at different latitudes reveals a dense array of narrow bands, cloudy “zones” and less cloudy “belts”. Many of the zonal bands are broken up by discrete cloud features.

The Equatorial Zone on the contrary, is a region of maximum vertical extent of the upper tropospheric haze and it is evident that the image at near $5\ \mu\text{m}$ do not show this region to be populated with convective clouds. Rather, the haze is more uniform, possibly because of strong zonal wind shear.

Because the different rotation with latitude, in the boundary between the equatorial zone and the low latitudes near $\pm 10^\circ$ some elongate and oblique cloud structures seem to go inside the equatorial regime, playing (without any physical comparison however) the role that the trades-winds play on Earth. This is well visible in both hemispheres in the middle panel of Figure 4.8.

The asymmetry and the equatorial regime is well visible in the third panel as well. The RGB image, artificially saturated in order to make visible the three distinct regimes shows the thermal emission of the reddish northern hemisphere (red is at $5.06\ \mu m$) and the reflected sunlight regime at southern (blue at $1.26\ \mu m$). At the equator, is evident the change in regime.

Here, a strongly scattering green belt (green at $1.47\ \mu m$) shows the high optical thickness of the atmosphere.

This third observation and the Equatorial Zone regime is the last we plan to test the model.

We remark that our choice has been obviously influenced by the need to write down this thesis.

Instruments on Cassini however, continue to acquire data and much of the existing Cassini data has yet to be comprehended. In the coming years we can expect to gain a much better understanding of the details of seasonal change.

Images of Saturn's limb especially at high spatial resolution will provide detailed vertical profiles of the stratospheric haze. Additional stellar and solar occultations will yield detailed profiles and compositional information on the stratospheric haze as well. Ultimately we can expect these new data and analyses to illuminate the important chemical and physical processes which take place over many scales in space and time [12].

The Cassini observations continue to the present and planning is underway to extend the mission to northern summer solstice in 2017.

Data analysis and results

The Cassini mission has provided a series of observational constraints that any model should satisfy.

Models of the atmospheres of the gas giant planets have fast progressed in a short time, due both to an emerging understanding of the required physics and an increases in computing power.

Many model simulations however, are sometimes limited in their diagnosis of the vertical aerosols and clouds distribution and the need to explore different assumptions about the cloud microphysics is evident.

Future modeling studies would benefit from the further use of cloud-resolving models and should propose observables that would be indicative of the mechanisms at work on the gas giant atmospheres as input for the remote sensing community to develop an effective strategy for future exploration.

This chapter presents the preliminary results of the application of our model to the VIMS data described before. It provides also a brief discussion of the results comparing them in relation to similar studies.

5.1 VIMS - Model comparison

After the explanation of the model and the choice of the images, the final comparison is here presented.

In order to obtain informations about the vertical aerosols and clouds distribution and derive physical parameters from the comparison with the model, the analysis of acquired spectra can be separated in two different spectral ranges of the infrared instrument channels: the solar part, ranging between $1.0\ \mu m$ and $3.2\ \mu m$ and the thermal part, ranging between $4.4\ \mu m$ and $5.2\ \mu m$.

The evaluation of the VIMS-Model comparison is performed mainly in these two wavelength intervals for each of the three images. For every comparison, the dashed line at the bottom represent the lower limit in radiance where the fitting procedure is not applied. All the images are visualized in radiance units with a linear and independent stretching procedure, in gray scale color.

In the following paragraphs we present the comparison between synthetic spectra and

averaged VIMS spectra.

For every images, we define a region of interest (ROI).

A ROI is a generic set of single pixels of an image representing a relatively uniform area of the observed atmosphere.

For every ROI we consider one spectrum only, obtained as the average of all the single pixel spectra considered in the region of interest. This is valid for all three images.

Plots are obtained comparing the spectrum of the ROI with the estimated best fit spectrum of the spectral databank, both in the solar and thermal part.

As described in the chapter 4, the comparison provides some physical and optical parameters of the aerosols distribution used in the model to obtain the best fit with the observation.

To test the model we consider again the images chosen in the previous chapter, starting from the South Polar Region.

5.1.1 South Polar Region

We said that the two images of Figure 4.2 show the South Pole of Saturn at different wavelengths, revealing the opacity of the overlying stratospheric and tropospheric haze by its ability to block upwelling thermal radiation if seen at near $1.0 \mu m$. On the other hand, the thermal emission of the planet itself can be revealed by the presence of deeper clouds, if seen at $5 \mu m$.

Moreover, we explained the reason of the choice of this particular image.

In the bottom of the thermal image in fact, a semi-circular long bright cloudy feature is well visible.

This feature, seems to be split in two part.

The first one, is located near -72° latitude from left-bottom to the center of the bottom where is broken by a cloud free region, always near the same latitude, the second begins at near -74° from the center of the bottom of the image continuing all along the same latitude until the right side.

If we consider only the first of these two structures, we can see in the image that before the dark gap located at near -73° there is a gray lane extending just beside the arm. This should indicate the top of another cloudy system of relatively lower opacity with respect to the previous one.

Then, the dark and cloud free gap, revealing the thermal emission of the planet.

These three different atmospheric conditions present in the image are the regions chosen for the test.

In Figure 5.1, three ROIs are overlaid on the images, in order to show the three different region described before.

For every region, the pixels cover an uniform area in terms of radiance level.

This is due to the need to have a single spectrum for every ROI, averaged between the single pixel spectra, with small deviations between them.

In red, the region with high opacity where a dense deck of clouds is visible. The pixels cover an "arm" of the structure along the same solar incident angle.

In green, the pixels cover a part of the gray lane parallel the previous deck of clouds with the same *criteria* of uniform brightness and in blu the hot thermal cloud free region, where the escaping of the planet's internal heat occurs.

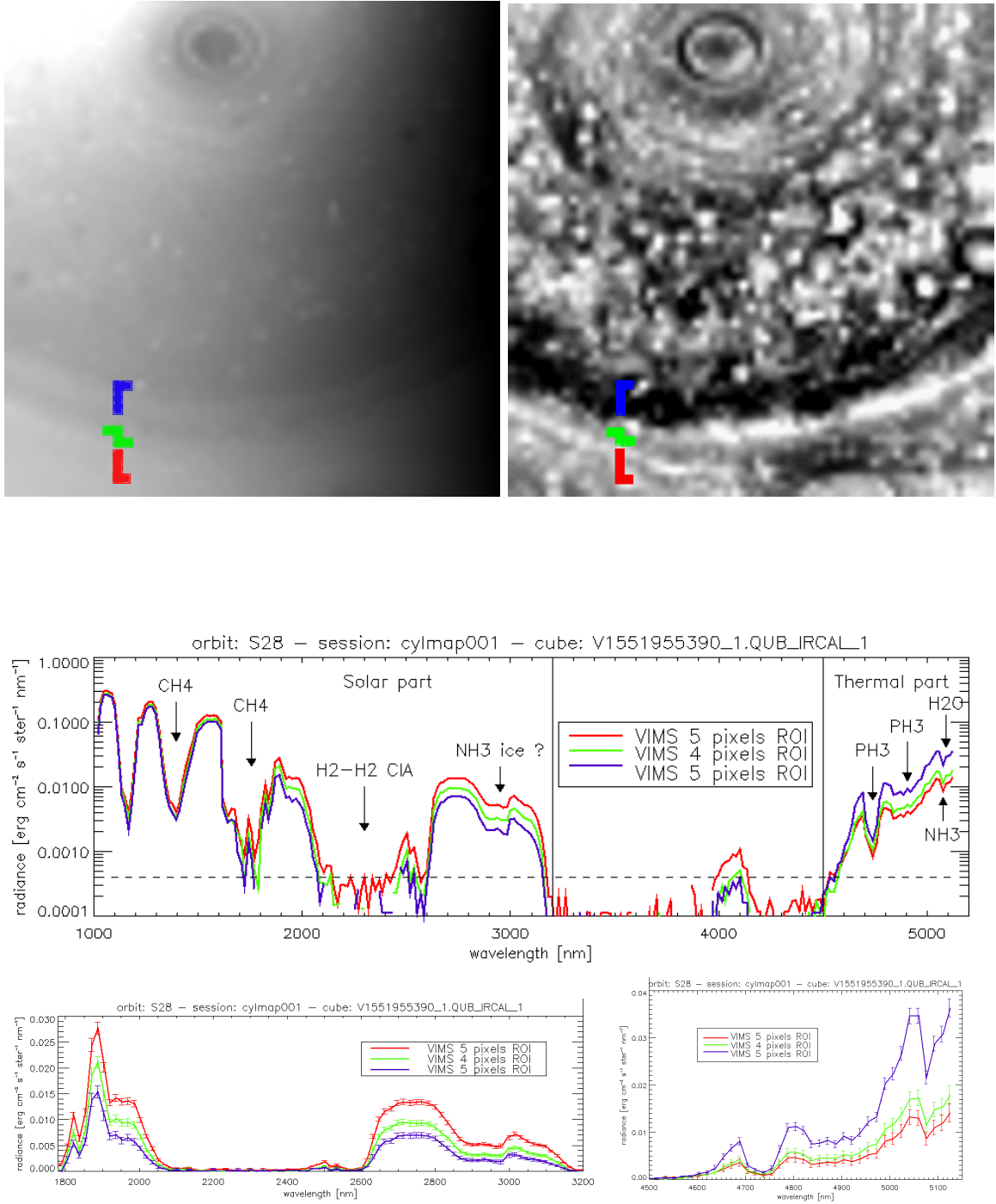


Figure 5.1: Same images of Figure 4.2 with overlaid the three ROI chosen for the comparison with the model. In the plots, the three different spectral behaviors are shown with the known spectral signatures.

The pixels have been chosen in order to satisfy two main conditions: all the pixels had to have the same solar illumination angle, in order to exclude any differences in the spectra due to the solar component (the pixels are illuminated in the same manner) and then the pixels had to cover different regions being all in near nadir emission angle. The difference between the higher emission angle and the smaller one is near 4° .

The position of the pixels and the ROIs is shown in the left picture of Figure 5.1. Here, the $1\ \mu m$ view shows a change in the haze regimes at the same latitudes. For this image the same conditions are respected as well.

What we said about the diversity of the chosen areas, is well visible in the plots of the acquired instrument spectra on bottom of the Figure 5.1.

Here two plots are presented.

The plot on top shows the entire instrument range spectrum for every ROIs¹. In the other two plots, a zoom of the range between $1.8\ \mu m$ and $3.2\ \mu m$ and of the thermal range between near $4.4\ \mu m$ and $5.2\ \mu m$ is shown.

The plots show the behavior of the three different regimes.

In the solar part, the red ROI scatters more sunlight with a relative high radiance signal due to the overlying diffuse haze visible in the $1\ \mu m$ picture on left of Figure 5.1.

In the thermal part however, the opposite effect is true, a dense cloud deck, well visible in the image at $5.1\ \mu m$ on the right of the same figure, blocks the thermal emission of the planet revealing a lower radiance signal between $4.4\ \mu m$ and $5.2\ \mu m$. For the green ROI, the haze is still scattering the sunlight but now, a lower opacity of the clouds is needed to explain the differences in the signal. In this case, in the solar part until and in the $3\ \mu m$ range, the plot shows differences with the red spectra revealing a different clouds structure. This is also evident in the thermal part where the thermal radiation level begins to arise.

The blu ROI shows the opposite behavior of the red one, here the depletion of aerosols affects the signal in the solar part, where the low number of scatterers produces the lower signal. In the thermal part however, the clouds relative absence allows the escaping of the radiation.

Spectral signatures of gaseous specie absorption also are shown. The VIMS spectra don't exhibit however the ammonia ice spectral feature around the $2.95\ \mu m$ as discussed in the model explanation.

In the following, for every single ROIs the results and discussion of VIMS-Model comparison is presented.

Model results: red ROI

The first thing we notice in the outputs of our model is how we always need to take into account for an optically thin stratospheric haze.

In order to fit the instrument spectra in fact, the model put the base of this stratospheric haze at $30\ mbar$ with particles radius $r_{eff} = 0.1\ \mu m$ and a total opacity τ_{haze} ² at $5.1\ \mu m$ of $4.1 \cdot 10^{-5}$.

This is the true for all three ROIs.

As explained in the paragraphs about the model, the stratospheric haze level is more responsible between the $1\ \mu m$ and the $2.5\ \mu m$ for the raising of the methane absorption bands bottom in terms of radiance levels with respect to the ammonia tropospheric

¹For simplicity, here and in all the other plots, every spectrum has the same color of the correspondent ROI for a quick look.

²We use the symbol τ_{haze} to indicate the total opacity of the stratospheric cloud level, τ_{tc} for the tropospheric cloud and τ_{dc} for the deep cloud opacity.

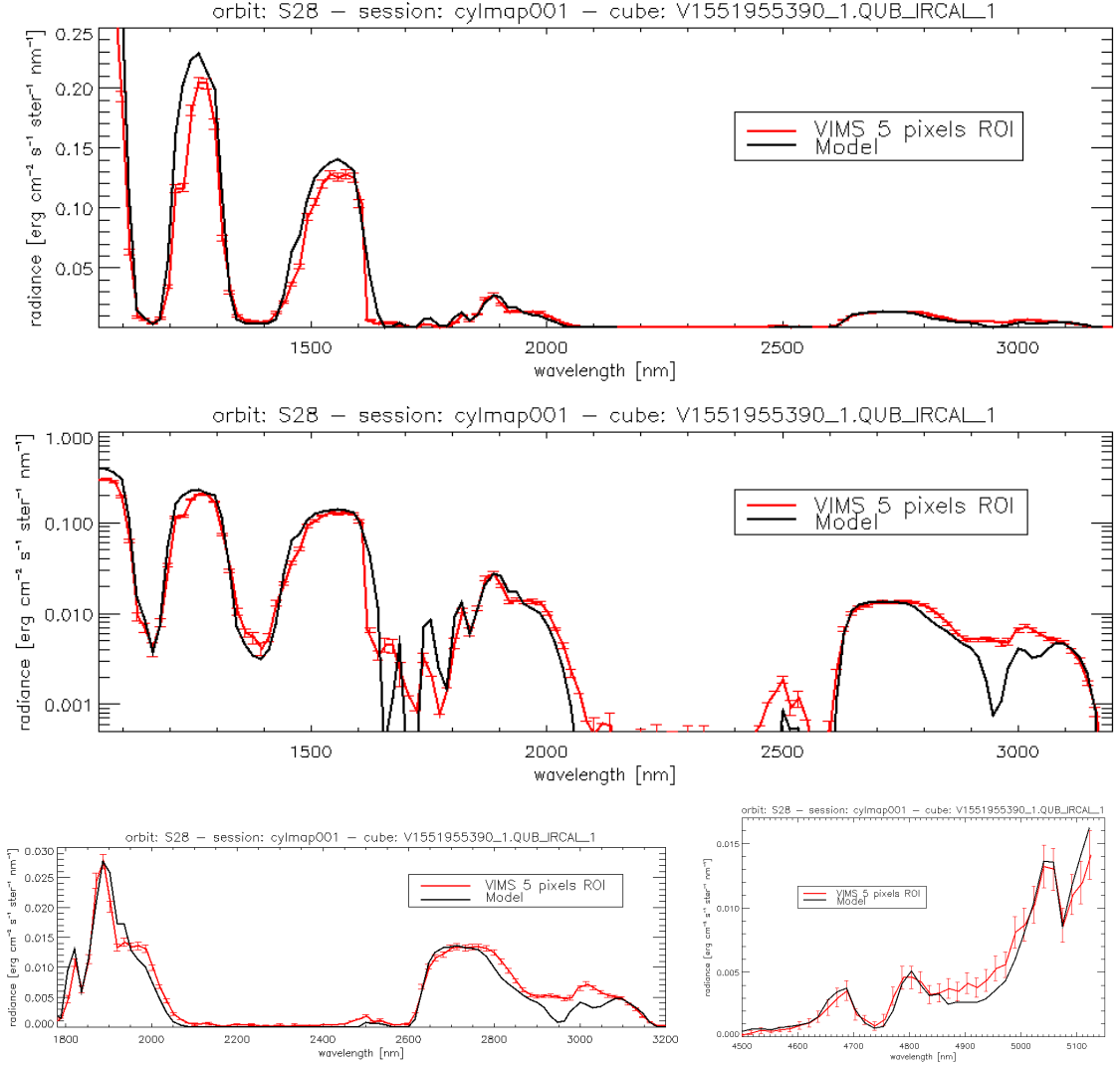


Figure 5.2: *VIMS-Model comparison for the red ROI of the South Polar Region. The panels on top and in the middle show the comparison in the solar part in linear and logarithmic scale respectively. On bottom, a spectral zoom of the comparison closer to 3 μm and in the thermal range is shown.*

clouds.

This means that a diffuse sheet of haze covers the entire region under observation and that there is no difference between the regions in the upper part of the atmosphere. Between the 1.8 μm and 3.2 μm range, shown on left-bottom of Figure 5.1, the situation is different. Here, the tropospheric clouds modulate the radiance level and the model predicts different physical parameters for the three regions.

This difference however, is in the pressure of the base of the clouds and in the total opacity only. The particles radius of the putative ammonia ice clouds in fact remains constant at the value of $r_{\text{eff}} = 0.7 \mu m$.

In the red ROI case, the comparison with the model gives for the tropospheric ammonia clouds a pressure level of 300 mbar and a total opacity $\tau_{tc} = 0.24$ at 5.1 μm . For the thermal part, the best fit is obtained with an optically thick cloud deck with the base located at pressure between the 2 bar and the 3 bar with $\tau_{dc} = 1.76$ for the

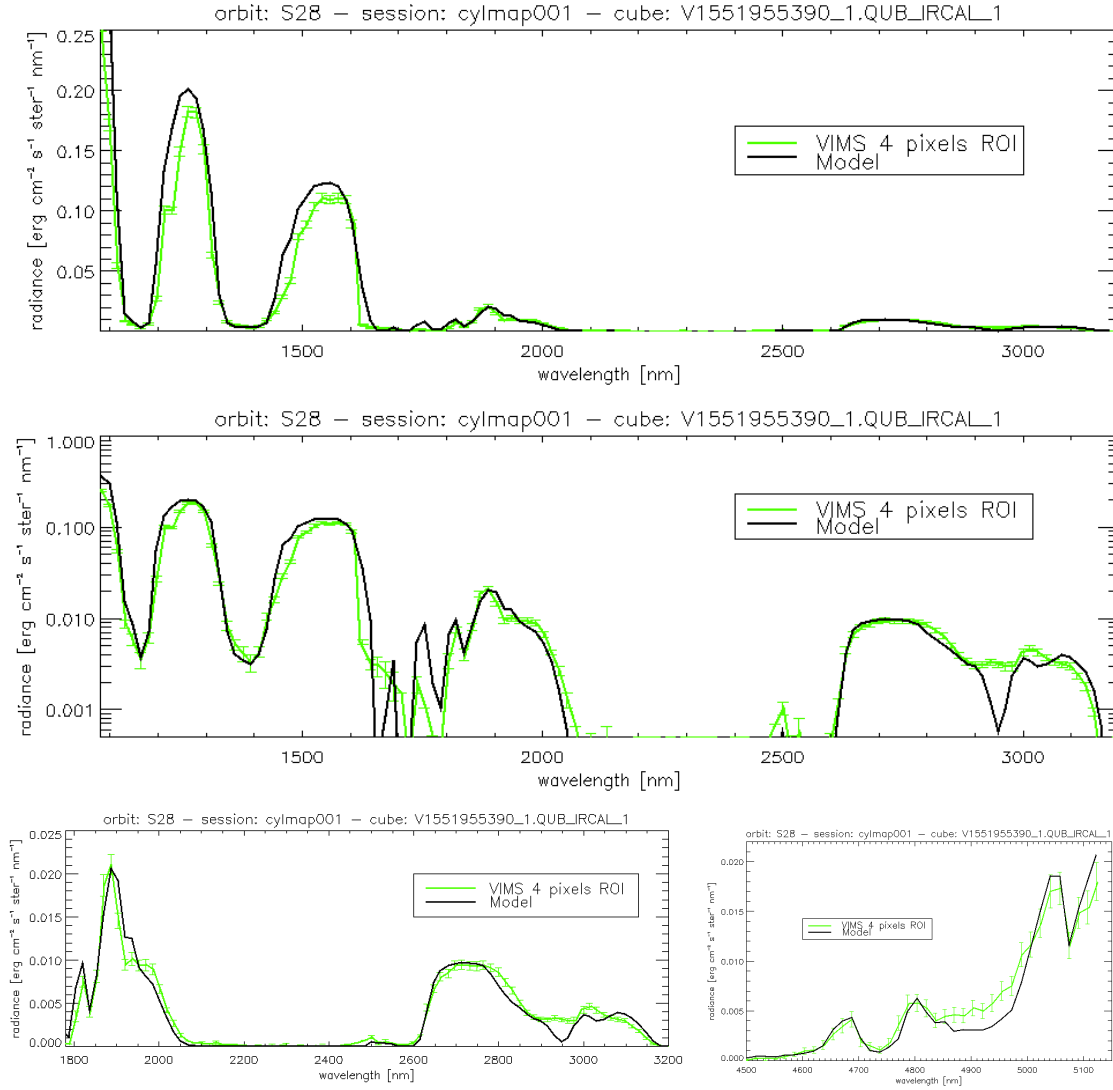


Figure 5.3: *VIMS-Model comparison for the green ROI of the South Polar Region.*

value of total opacity.

The Figure 5.2 shows the comparison between the VIMS spectrum and the model for the red ROI.

In the plot on top and in the middle of the figure, the comparison in the solar part between $1.0 \mu\text{m}$ and $3.2 \mu\text{m}$ is shown in linear and logarithmic scale respectively.

The model can't fit the methane windows at near $1.25 \mu\text{m}$ and $1.55 \mu\text{m}$ and the portion of the spectrum between $1.65 \mu\text{m}$ and $1.85 \mu\text{m}$.

The strong ammonia ice spectral signature at $2.95 \mu\text{m}$ is well visible in the model especially in the logarithmic scale plot but, as said before VIMS does not exhibit this feature.

In the thermal part, the model is not able to fit the spectrum in the range between $4.8 \mu\text{m}$ and $5.0 \mu\text{m}$.

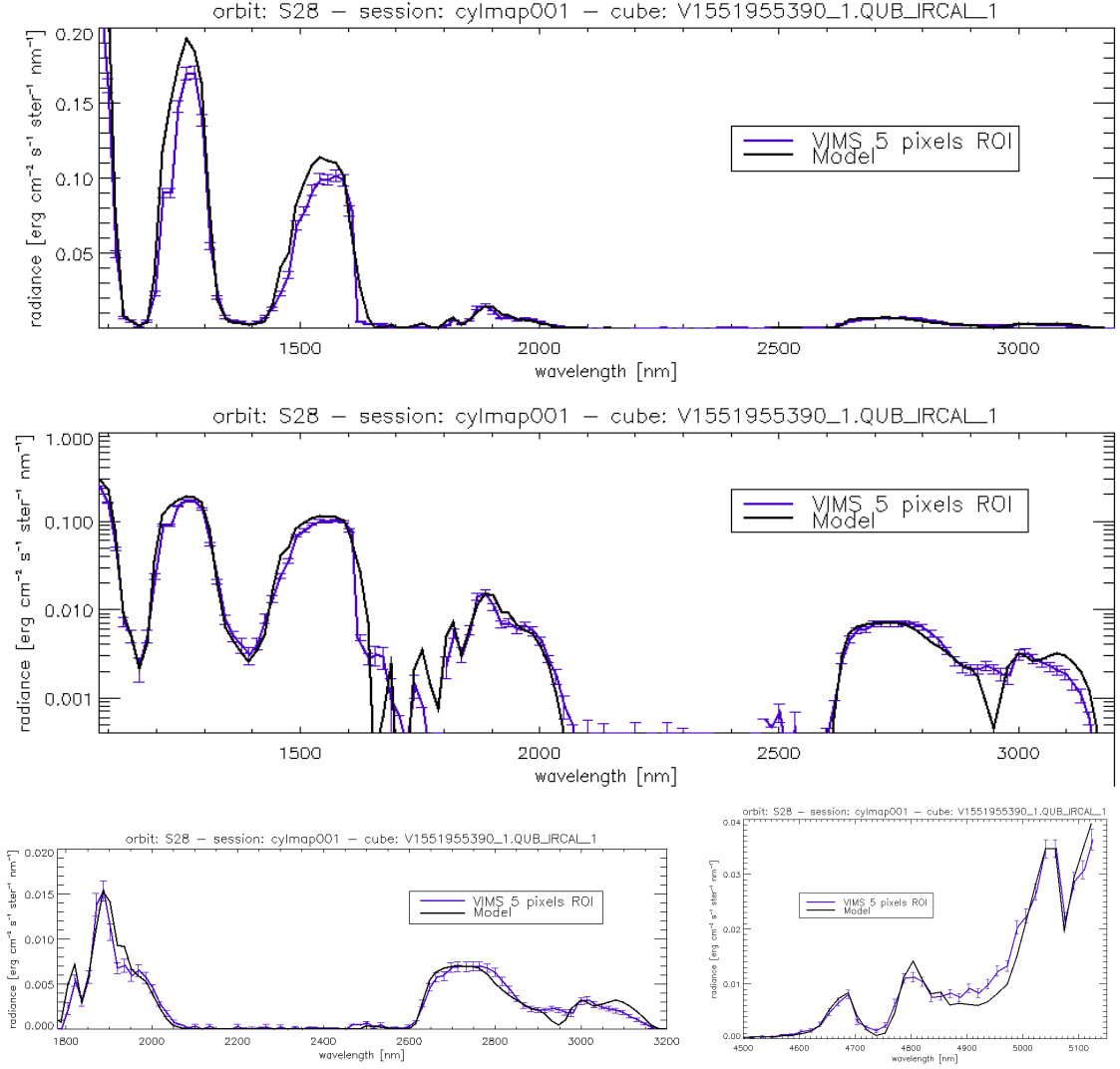


Figure 5.4: *VIMS-Model comparison for the blu ROI of the South Polar Region.*

Model results: green ROI

In the green ROI case, the comparison with the model gives for the tropospheric clouds base a pressure level of 350 *mbar* with a total opacity $\tau_{tc} = 0.15$ at 5.1 μm .

For the thermal part, the best fit is found with a deep cloud with the base located at pressure between the 3 *bar* and the 3.5 *bar* with an opacity $\tau_{dc} = 1.5$.

This values show how the model predicts a tropospheric cloud located at lower altitudes but thinner with respect to the red case and a deep cloud with less opacity located deeper in the atmosphere.

The Figure 5.3 shows the results for this ROI. Here again is impossible for the model to fit the windows and the same differences between the model and the actual acquisition are clear.

Anyway the model fits the 3 μm region of the spectra and the thermal part in a better way.

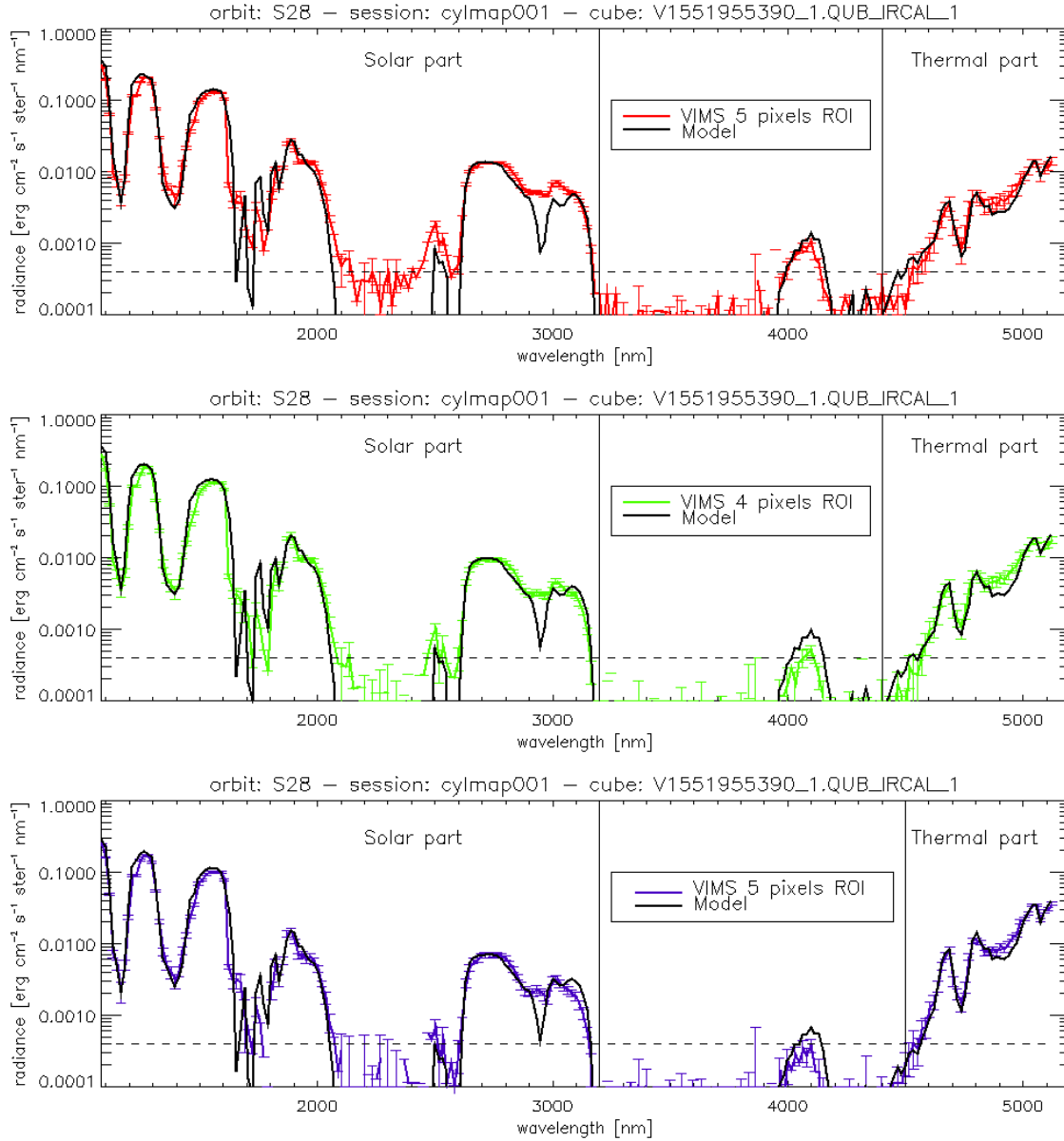


Figure 5.5: All range VIMS-Model comparison for the three ROIs of the South Polar Region.

Model results: blu ROI

What we retrieve in this case is that the ammonia ice cloud is located at 400 *mbar* with a total opacity $\tau_{tc} = 0.09$ and a deep cloud with $\tau_{dc} = 0.56$ located below the 4 *bar* level.

In this last case however, the positioning of the deeper cloud is not well determined because the model is not able to give a defined interval of pressures where the fit occurs but it seems more that below the 4 *bar* level it gives the same result in terms

South Polar Region			
Nominal aerosol/cloud	pressure [mbar]	r_{eff} [μm]	τ_{cloud} (at 5.1 μm)
red ROI:			
Stratospheric haze (N ₂ -CH ₄ ice)	30	0.1	$4.1 \cdot 10^{-5}$
Tropospheric cloud (NH ₃ ice)	300	0.7	0.24 ± 0.03
Deep cloud (NH ₄ SH ice)	$2 \div 3 \cdot 10^3$	40	1.76 ± 0.16
green ROI:			
Stratospheric haze (N ₂ -CH ₄ ice)	30	0.1	$4.1 \cdot 10^{-5}$
Tropospheric cloud (NH ₃ ice)	350	0.7	0.15 ± 0.02
Deep cloud (NH ₄ SH ice)	$3 \div 3.5 \cdot 10^3$	40	1.5 ± 0.12
blu ROI:			
Stratospheric haze (N ₂ -CH ₄ ice)	30	0.1	$4.1 \cdot 10^{-5}$
Tropospheric cloud (NH ₃ ice)	400	0.7	0.09 ± 0.02
Deep cloud (NH ₄ SH ice)	$> 4 \cdot 10^3$	40	0.56 ± 0.05

Table 5.1: *Clouds parameters for the VIMS-Model South Polar Region comparison.*

of fit with the observation.

Figure 5.4 shows the plots of the comparison between the VIMS data and the model. There is a good agreement in the bottom of the methane absorption bands between the spectra. The simulation before near 3 μm is good before the ammonia ice signature then the fit is lost. The thermal part shows a good agreement with the actual data as well.

Figure 5.5 shows for the three regions of interest, the comparison between the VIMS averaged spectra and the model simulations. Every simulated spectrum is obtained with the parameters of Table 5.1 and represents the best fit in all the instrument spectral range between 1 μm and 5.2 μm .

5.1.2 Middle Latitudes

The mid-latitudes of the southern hemisphere we consider were observed by Cassini on February 2008 when the spacecraft was at 800.000 km from the planet.

Figure 4.5 of the previous chapter shows the mid-latitudes of the planet from -50° to -80° .

In Figure 5.6, the images taken at 1.06 μm and 5.06 μm are shown, with the last one photometrically inverted.

Here again, three different ROIs are overlaid on the images covering three different cloud conditions.

The reason of this choice is due to the fact that the red and the green ROIs cover the same regime when we look at the 1 μm image on the left. Here, at a latitude of near -55° a diffuse haze cover the entire mid-latitudinal zone.

Looking at Figure 4.7 we notice that both ROIs have the same solar illumination angle and are pretty close in latitude to minimize any difference in the spectra due

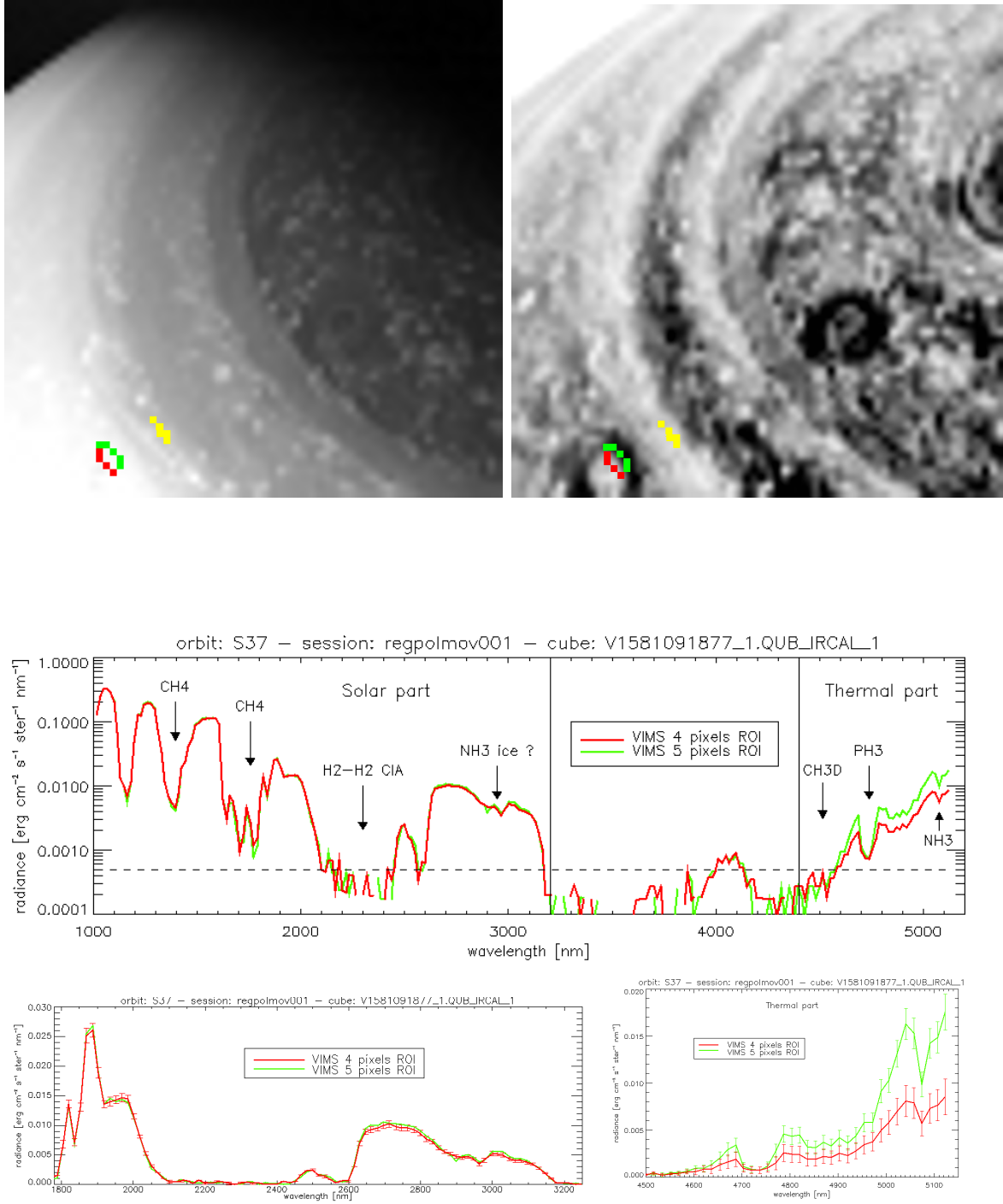


Figure 5.6: South Middle Latitudes images with the three ROIs chosen. In the plots, the different spectral behaviors for the green and the red ROIs are shown. For the yellow ROI see Figure 5.9.

to the different path of the reflected sunlight.

Moreover, the ROIs are located before the -60° , where the behavior of aerosols and clouds begins to change, in order to be sure that the regime of upper part of the atmosphere is the same for both ROIs.

In the $5.06 \mu m$ image on right of Figure 5.6, the deeper layers sounded at that wavelength reveal a completely different scenario. Here, an *hot spot* structure is well visible, as mentioned in the chapter about the chosen VIMS images, with a cloudy structure located in the middle.

This is another reason of the choice.

The red and green pixels cover an area that is very similar in the solar part but completely different in the thermal, giving a good opportunity to test the model before the aerosols regime change at near -60° .

Because this change occurs near that latitude, another ROI is taken after that to test the validity of the model. In the same figure in fact, is visible a yellow ROI located at -60° .

The RGB image on left in Figure 4.6 shows very well this change and we can see how the red and green ROIs are inside the same regime and how the yellow ROI covers a different spectral behavior.

The blu color intensity changes at that latitude and it is clear how, in respect with the previous reasons about latitude, incident and emission angle, the yellow ROI is located at the changing behavior closer region.

If we look now at the plots below the images in Figure 5.6, the spectral behavior mentioned before about the ROIs is evident. In the solar part, the red and green spectra are almost identical and they differ only in the thermal range because their different deeper layers structures.

As before, for every single ROIs the results and discussion of VIMS-Model comparison is presented next.

Model results: red ROI

The similarity of the red and green ROIs in the solar part of the wavelength range, is evident in the simulated spectra as well.

In Figure 5.7 the comparison between instrument and model for the solar part is shown using only the spectrum of the red ROI, being equal to the green one in that particular range.

Even the range $1.8 \mu m \div 3.2 \mu m$ is fitted by the same simulation as shown in the two plots at left.

Here again, an unique layer of stratospheric haze is enough to fit the bottom of the methane bands and the spectral region near $1.8 \mu m$.

For all three ROIs we found that the stratospheric haze is located at higher altitude with respect to the southern regions, being the haze's base pressure level located at $20 mbar$. But now, the change of aerosols regime is highlighted by the change in radius of the particles.

The model needs a value of $r_{\text{eff}} = 0.12 \mu m$ to fit the signal coming from the red and green ROIs. So, the correspondent opacity at $5.1 \mu m$ is fixed at $\tau_{\text{haze}} = 1.5 \cdot 10^{-4}$.

For the tropospheric cloud the model needs a change in the properties of the particles of ammonia ice.

Here, particles with radius $r_{\text{eff}} = 0.75 \mu m$ give the best fit with the observations. The clouds base is located at $350 mbar$ with an opacity of $\tau_{tc} = 0.11$ for both the regions. The thermal part, however, differs for the presence of the cloudy structure inside the

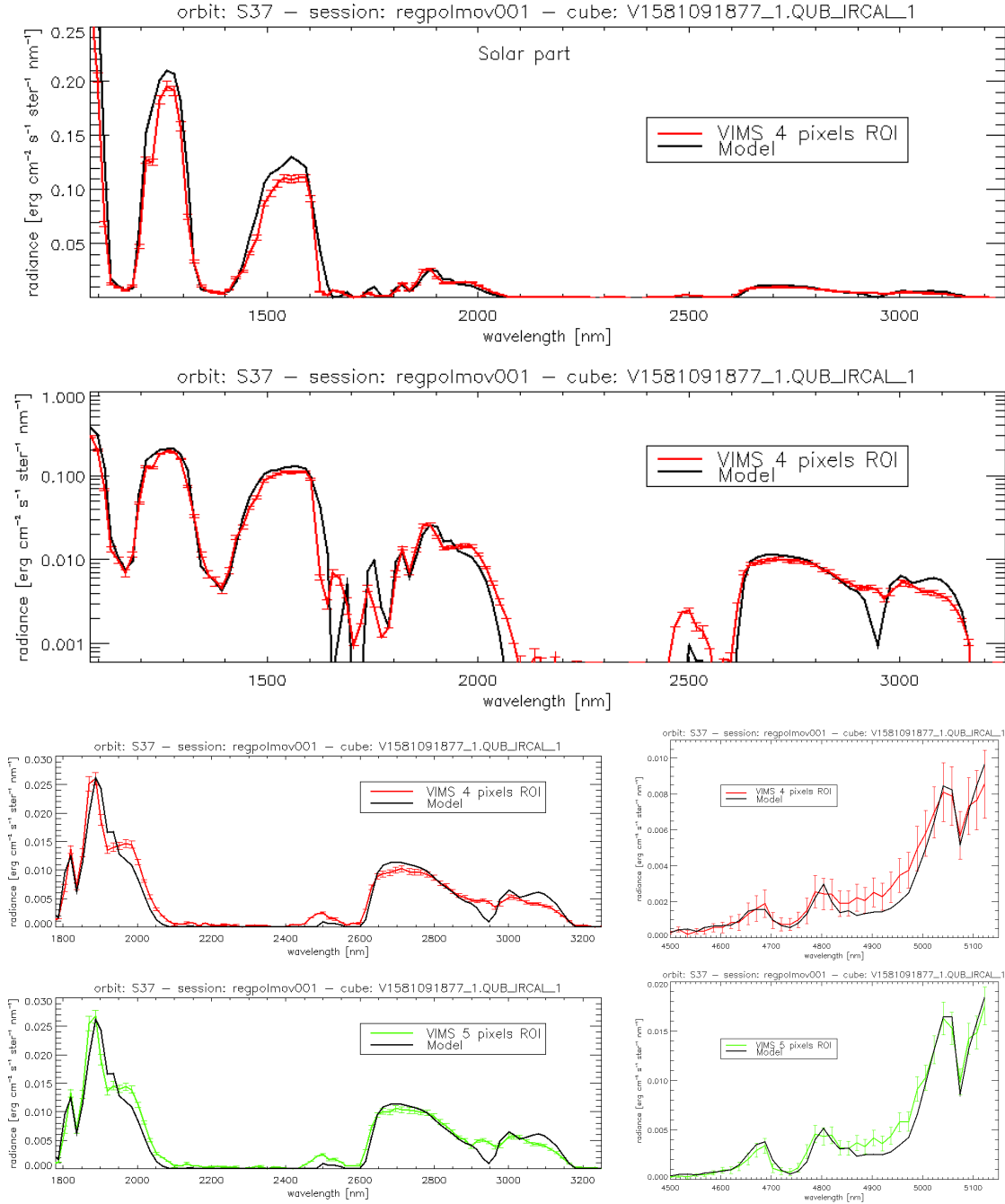


Figure 5.7: VIMS-Model comparison for the red and green ROIs of the South Middle Latitudes. In this case only the thermal part is different between the spectra. The solar part can be simulated by the model with the same parameters for both the red and green ROIs.

hot spot for the red ROI. In this case, a deep cloud deck must be located at 2 bar with $\tau_{dc} = 2.46$ in order to fit the instrument spectrum.

In Figure 5.7 the comparisons for the red ROI in the range between 1.8 μm and 3.2 μm and for the range 4.4 μm and 5.2 μm are also shown.

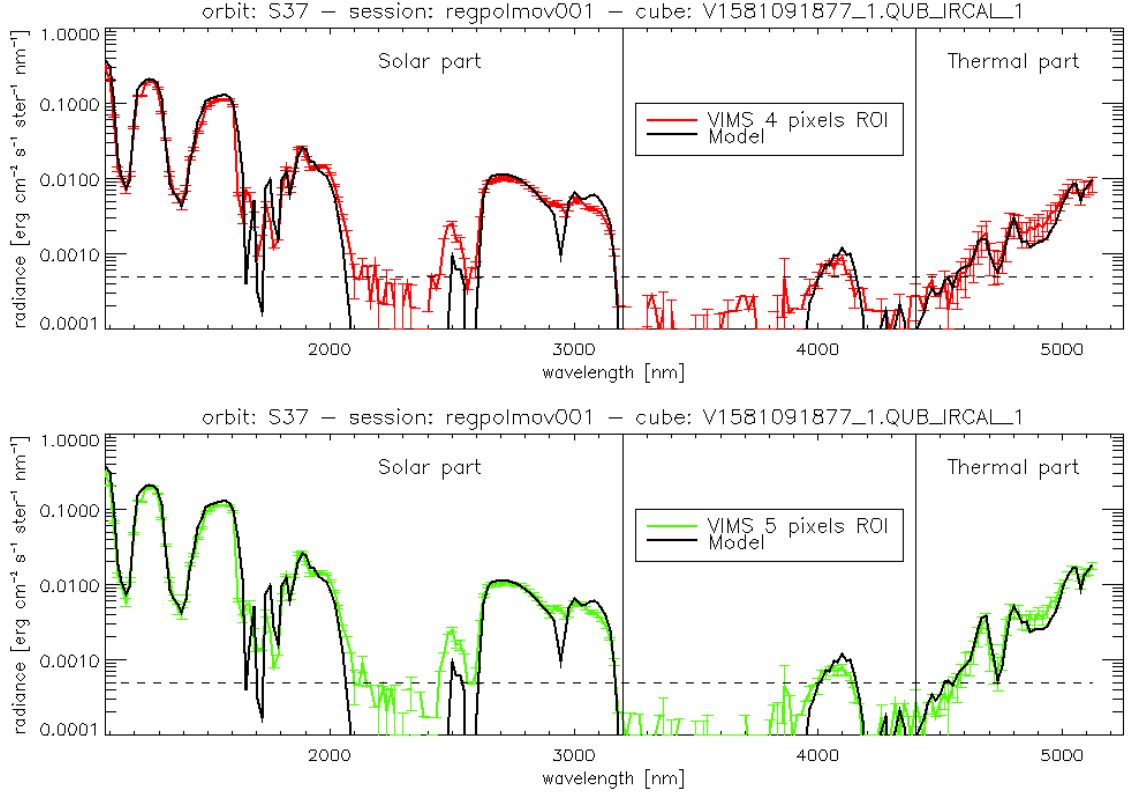


Figure 5.8: *All range VIMS-Model comparison for the red and green ROIs of the South Middle Latitudes.*

Model results: green ROI

For the green ROI, all the comments for the red one about the solar part of the model are basically the same.

For the stratospheric and tropospheric clouds the parameters used for the simulation are the same and the only difference is in the thermal range.

Here, in order to fit the data the deep cloud deck needs to be placed at deeper levels with different opacity. The cloud base pressure is at 3 bar with an opacity of $\tau_{dc} = 1.56$, always at $5.1 \mu m$.

Below the plots for the red ROI, the comparison in the same spectral ranges for the green one is shown in the same figure.

In Figure 5.8 the all range comparison of the red and green ROIs is shown.

Model results: yellow ROI

For the third ROI we found that the best fit occurs if we use again the value of $0.7 \mu m$ for the tropospheric particles radius r_{eff} .

The change in aerosols regime at -60° is confirmed by the minor total opacity of the tropospheric cloud, where the model predicts a value of $\tau_{dc} = 1.56$ and a pressure of 400 mbar.

Looking at the Figure 5.9, this behavior is evident, the solar part exhibits a lower

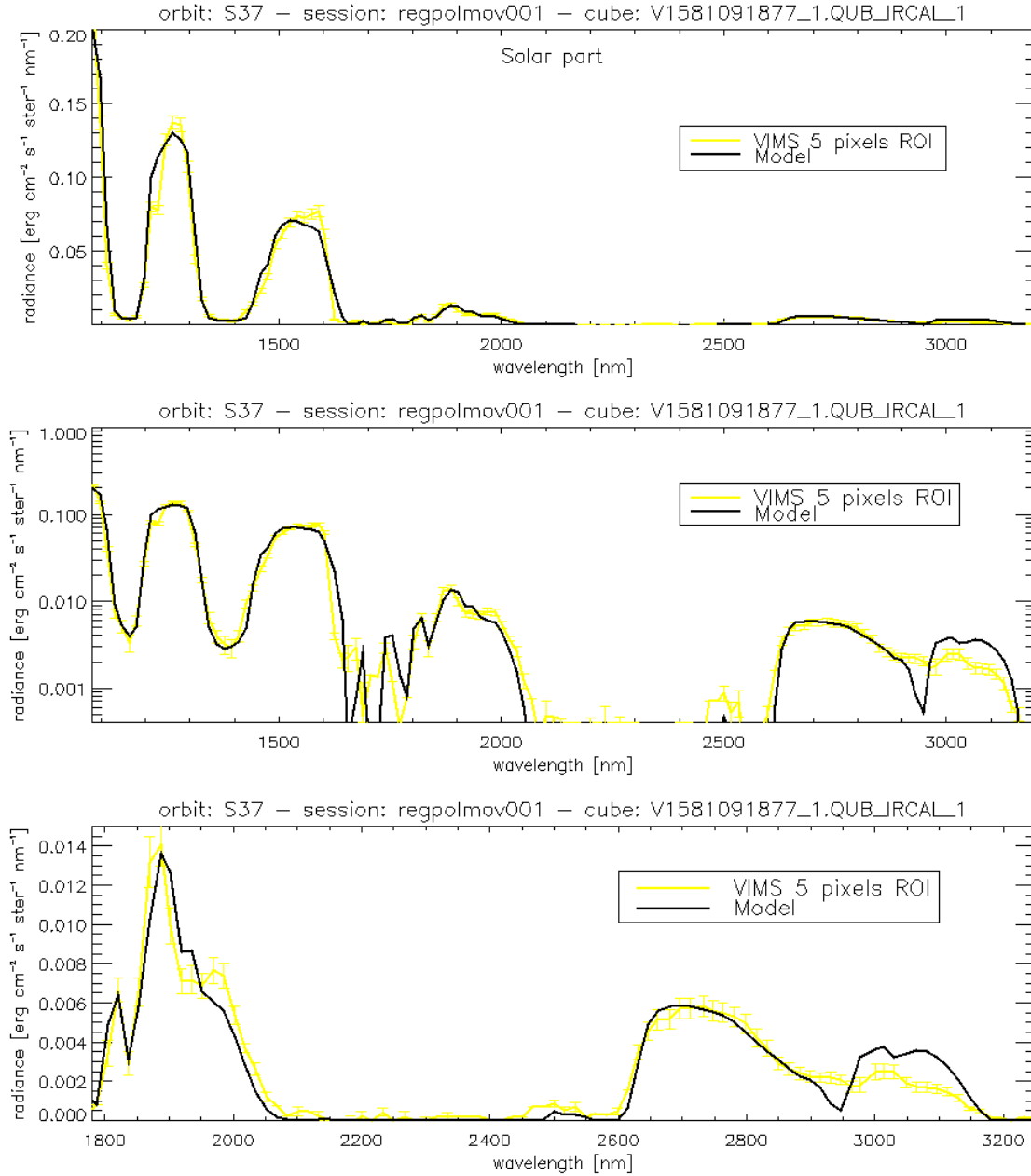


Figure 5.9: *VIMS-Model comparison for the yellow ROI of the South Middle Latitudes*

radiance signal. In this case, in order to fit the bottom of the methane bands, the simulation lost fit with the windows where the signal is higher than the simulated one.

In this case is not possible to fit the thermal part. The simulation in fact, because of relatively high opacity of the simulated deep cloud in order to fit the thermal spectral range, lost the shape of the phosphine absorption bands at near 4.75 μm and near 4.9 μm , making the comparison impossible.

However we prefer to omit the comparison in this case.

South Middle Latitudes				
Nominal aerosol/cloud		pressure [<i>mbar</i>]	<i>r</i> _{eff} [<i>μm</i>]	<i>τ</i> _{cloud} (at 5.1 <i>μm</i>)
red ROI:				
Stratospheric haze	(N ₂ -CH ₄ ice)	20	0.12	1.5 · 10 ⁻⁴
Tropospheric cloud	(NH ₃ ice)	300	0.75	0.11 ± 0.01
Deep cloud	(NH ₄ SH ice)	2 ÷ 2.5 · 10 ³	40	2.46 ± 0.26
green ROI:				
Stratospheric haze	(N ₂ -CH ₄ ice)	20	0.12	1.5 · 10 ⁻⁴
Tropospheric cloud	(NH ₃ ice)	300	0.75	0.11 ± 0.01
Deep cloud	(NH ₄ SH ice)	3 ÷ 3.5 · 10 ³	40	1.55 ± 0.26
yellow ROI:				
Stratospheric haze	(N ₂ -CH ₄ ice)	30	0.1	4.1 · 10 ⁻⁵
Tropospheric cloud	(NH ₃ ice)	350	0.7	0.04 ± 0.004
Deep cloud	(NH ₄ SH ice)	-	-	-

Table 5.2: *Clouds parameters for the VIMS-Model South Middle Latitudes comparison.*

5.1.3 Equatorial Zone

The third and last image used for the comparison is relative to the Equatorial Zone. In this case, the aerosols and clouds regime is definitely different. As pointed out in the previous chapter, the tropical band is the place where the largest scattering densities are present.

The central panel in Figure 4.8, shows the entire planet body as mosaiking of three different observations. The image at 5.1 μm on right in the Figure 5.10 shows the central cube of that mosaiking and it is evident the absence of any discrete cloudy structures and the almost total homogeneity of the radiance level.

In respect with the other observations, the Equatorial Zone exhibits an aerosols and clouds regime completely different, where the high and uniform opacity of the atmosphere is well visible.

In the left image at 1.06 μm in the same figure, a light change in the regime between the edges of the equatorial band in the northern and southern hemispheres near $\pm 10^\circ$ is still visible.

Again as before, a region of interest has been considered. Here, the red ROI is a five pixels area and is located just below the Rings. The reason of the choice is related to the need for the usual almost nadir view and to consider the inner part of the equatorial band in order to avoid any influence by southern hemisphere.

Looking carefully at both the images, it is clear that there is a gap between the faint dark line representing the Rings and the ROI. The atmosphere is still visible. The reason of the gap can be explained considering that we wanted to avoid any influence to the ROI spectrum by the signal coming from the Rings.

To better understand the different of the radiance signal in the Equatorial Zone, we can look at the plot below the two images.

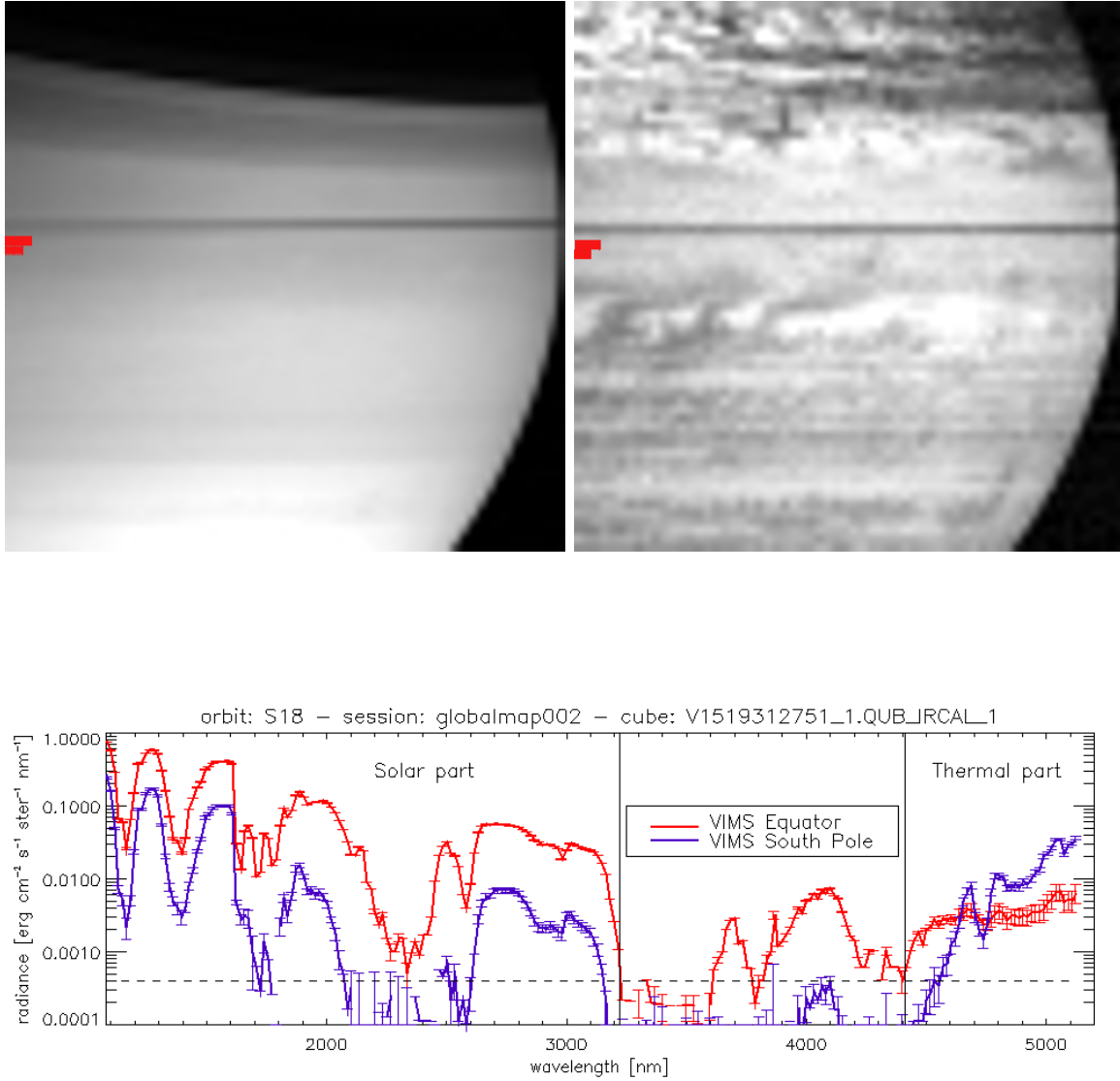


Figure 5.10: *Equatorial image of Saturn with the overlaid red ROI chosen for the comparison with the model. In the plot, the very different spectral behaviors of the Equatorial Zone and the South Pole Region as acquired by VIMS, are shown.*

Here, the ROI averaged spectrum is compared to the blu ROI spectrum of the South Polar Region discussed before. The comparison shows the huge difference, in terms of intensity of radiance and spectral behavior.

In the solar part, it is evident the presence of strong scatterers. From $1.0 \mu\text{m}$ to $3.2 \mu\text{m}$ the red signal is near an order of magnitude with respect to the blu one. After this range and before the thermal part, the signal coming from the blu ROI of the South is under the limit of the fit while the red spectrum is well above.

In the thermal part, the diversity of the nature of the atmospheric regime is evident looking at the spectral behavior of the red line. The atmospheric high opacity seems to crush the spectrum, making the shape of the absorption bands change.

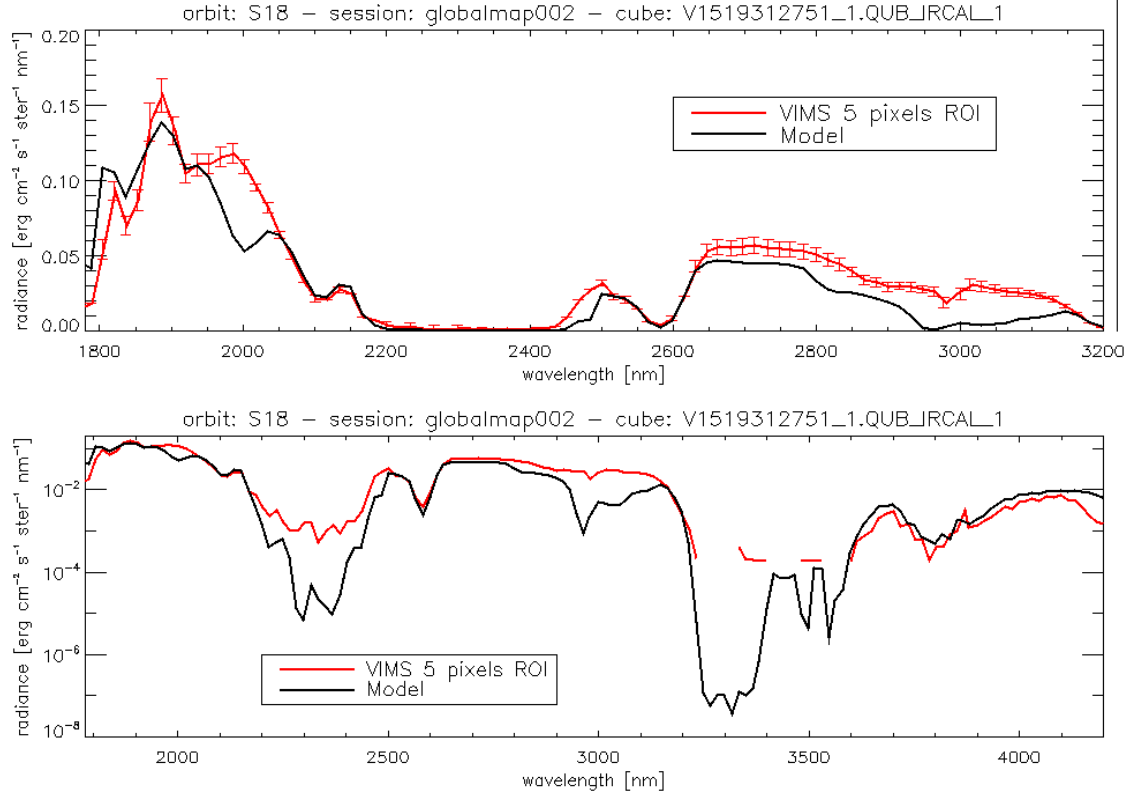


Figure 5.11: *VIMS-Model comparison for the Equatorial ROI. In this case the model is not able to reproduce all the signal of VIMS but only in the $1.8 \mu\text{m}$ to $4.2 \mu\text{m}$. In the upper plot the usual view at near $3 \mu\text{m}$.*

Model results: red ROI

Such diversity is still evident in the code outputs...

The model is not able to fit the data.

We have not found a good compromise for all the spectral range. It was impossible to fit both the solar and thermal part. The only part of the spectrum that we have tried to simulate with the model for the equatorial case however is the range between $1.8 \mu\text{m}$ to $4.2 \mu\text{m}$.

In Figure 5.11 the usual range near $3 \mu\text{m}$ and the total comparison are shown.

The plot on top shows how the level of VIMS radiance between $2.65 \mu\text{m}$ to $3.2 \mu\text{m}$ is lost. The model can't reach that level of signal and the part near $2 \mu\text{m}$. In the complete view below, the logarithmic axis shows better such differences.

The optical parameters used for the simulation however, reveal that the stratospheric haze in this case is made of particles of $r_{\text{eff}} = 0.2 \mu\text{m}$ with a base cloud pressure less or equal to 5 mbar . The model can't distinguish over that limit and the total opacity of the haze is $\tau_{\text{haze}} = 4.6 \cdot 10^{-4}$.

The tropospheric cloud is located at 200 mbar with particles radius $r_{\text{eff}} = 2.0 \mu\text{m}$ and a opacity $\tau_{\text{tc}} = 13$ at $5.1 \mu\text{m}$.

The use of a deep cloud in this case has no sense, in Table 5.3 we report the value of the first two cloud decks only.

Equatorial Zone			
Nominal aerosol/cloud	pressure [<i>mbar</i>]	r_{eff} [μm]	τ_{cloud} (at 5.1 μm)
red ROI:			
Stratospheric haze (N ₂ -CH ₄ ice)	< 5	0.2	$4.6 \cdot 10^{-4}$
Tropospheric cloud (NH ₃ ice)	200	2.0	13.08 ± 3.6
Deep cloud (NH ₄ SH ice)	-	-	-

Table 5.3: *Clouds parameters for the VIMS-Model Equatorial Zone comparison.*

5.2 Discussion

After the comparison between our data and the VIMS ones, we can draw the conclusions about the three different regions of Saturn investigated.

It is evident how the model cannot give an unique solution but only the best combination of all the *a priori* parameters able to fit better the instrument spectra. We remark that the reported values in the Tables are only the parameters taken from the spectral databank that fit better every ROIs spectra.

South Polar Region

In Table 5.1 the optical parameters used to fit the South Polar Region are shown. We found that an uniform stratospheric haze covers all three regions of interest. This haze is located at near 30 *mbar* with particles having $r_{\text{eff}} = 0.1 \mu\text{m}$ of mean radius. With the same assumption of spherical particles for the stratospheric haze, other studies reveal a mean aerosol radius of 0.15 μm for the aerosols near the North Pole [36] and a range between 0.1 μm and 0.15 μm for South Pole, where the stratospheric particles are more absorbent at UV wavelengths poleward of -70° than at other latitudes [77].

Other studies give for the the haze a pressure level comprised between 1 *mbar* and 30 *mbar* [20] for the southern polar region.

The tropospheric cloud of the simulation is located at pressures ranging between 350 *mbar* and 450 *mbar* moving from the cloudy area (red ROI) to the cloudless one (blu ROI). Other studies model the bottom pressure of this cloud layer at near 400 *mbar* [77].

In the South Pole Region, a value of $\sim 1 \mu\text{m}$ for the particle radius of this cloud level is predicted [12], where our model gives a common value of $r_{\text{eff}} = 0.7 \mu\text{m}$ for the three ROIs.

All the three ROIs, show pretty similar behaviors in the tropospheric layers but differ in the thermal part. The red and green regions of interest seem to have more in common in the thermal part of the spectrum with respect to the blu one, where the radiance signal between the 4.4 μm and 5.2 μm is higher.

The simulation is in agreement with the images as well, where the red and green ROIs show more similarity in the level of radiance with respect to the blu one.

This is also shown by the different opacity of the deeper cloud for the three ROIs, as shown in Table 5.1.

South Middle Latitudes

The first variation of the properties of the stratospheric haze and tropospheric clouds take place at the latitudes near -60° .

In order to fit the VIMS spectra at that latitude, the model gives for the stratospheric haze an uniform set of parameters before the change near -60° for the red and green region of interest.

Here, particles of $r_{\text{eff}} = 0.12 \mu\text{m}$ give the best fit, with a base pressure of 20 *mbar*. Now, the particles are bigger and the haze is higher in altitude with respect to the South Pole Region. Similar quantities are found by other studies, that reveal how the stratospheric haze is situated between 10 *mbar* and 30 *mbar* with particles of 0.15 μm in radius [70].

Other studies predict a level below 10 *mbar* at these latitudes for the upper haze [48]. The same studies predict that the tropospheric cloud has to be located from 130 *mbar* to 600 *mbar*, where our model gives a value of 300 *mbar*. Other values are predicted from 80 *mbar* to 400 *mbar* for the same latitudes [34].

Looking at the values of Table 5.2 we note that the particles radius of the tropospheric cloud used for the best fit simulation is $r_{\text{eff}} = 0.75 \mu\text{m}$.

Studies of the evolution of Saturn's hazes and clouds during the 1991–1993 period using ground-based images in the red methane bands ($619 \div 948 \text{ nm}$) and in their adjacent *continuum*s use the same value for the tropospheric cloud particles radius [50].

In order to fit the yellow ROI spectrum, we need to change both the parameters of the stratospheric haze and the cloud below. The model reveals the change of regime putting the tropospheric cloud at higher pressure and lower opacity with respect to the values used in the red and green ROIs simulations.

The pressure top level and especially the optical depth variations with latitude of this haze and clouds are the most important factor in generating the visual appearance of the planet.

Equatorial Zone

In the Equatorial Zone the haze is thicker and higher than elsewhere on the planet. At most latitudes Saturn's zonal winds have been remarkably stable over time. The one major exception is the prograde equatorial jet. Measurements from the Voyager green filter images yield a peak zonal wind of 450 m s^{-1} [21].

Other studies found that winds measured by different HST filters sensitive to different altitudes at this time had different speeds, suggesting the presence of vertical shear in the zonal wind [31].

Observations at different wavelengths allow the detection of individual cloud tracers at different altitudes within this cloudy structure in the Equator.

The results show how these different altitudes change in time. Some studies suggest that the levels of these tracked equatorial cloud/haze features were placed at between 200 *mbar* and 500 *mbar* in the measurements of 1980–81 [21].

Images analysis of the Hubble Space Telescope in the 2004, indicates that tracers were placed high in the atmosphere at near 50 *mbar*. These results were confirmed

by the first reflectivity measurements and models of the equatorial zone performed in 2004 and early 2005 with Cassini-ISS instrument in the wavelength range from 250 nm to 950 nm [21]. Individual cloud elements were detected at two levels within the tropospheric cloud at 50 $mbar$ and deeper in the 700 $mbar$ level, representing a vertical shear of the zonal wind.

Even if our model fails the comparison with the observed spectrum in all the range of the instrument, the only portion between 1.8 μm to 4.2 μm is enough to retrieve some physical parameters. Table 5.3 shows such parameters.

The radius of the stratospheric haze is larger when compared to the previous ones. we found that the best fit occurs with a particles radius of $r_{\text{eff}} = 0.2 \mu m$. The haze, in this case, is located in the higher atmosphere, at near 5 $mbar$.

Our results are in agreement with the results obtained by other authors, an upper thin haze in the stratosphere is found to be persistent and formed by same particles radius in a pressure range between 1 $mbar$ and 10 $mbar$ [77].

The tropospheric cloud deck, however, is the main responsible for the high intensity level. Table 5.3 shows that the comparison gives a radius of the tropospheric particles of $r_{\text{eff}} = 2.0 \mu m$.

Extensively studies of the cloud structure and aerosol properties of Saturn's equatorial region at -10° latitude give a range of the tropospheric clouds radius from 0.5 μm to 2.0 μm with the lower boundary at pressures as low as 300 $mbar$ [83].

5.3 Conclusions and perspectives

In preparing our RT model we were well mindful of the relative simplicity of the model and how the final outputs of our code about the optical properties of aerosols and clouds were only the best configuration in order to fit the actual data.

We remark that the values of the final comparisons, not represent the actual atmospheric structure under observation but only the most similar configuration that could represent it, in the limit of our simplification.

It is difficult to directly relate aerosol optical properties derived from modeling to constraints on physical properties such as size of the particles. Thus, we do not consider the retrieved values for the physical properties of the aerosols as the actual values of particles in the atmosphere, but as a combination of parameters that can reproduce observational data.

Anyway, the aim of this thesis is the construction of a RT model which simulates the radiance of the image spectrometer VIMS of the Cassini Huygens mission to Saturn and to retrieve the best set of aerosols and clouds physical parameters in order to fit the signal of different observations.

The banded visual appearance of Saturn and the alternating pattern of jet streams with latitude, suggest a regional classification of the haze content in three main bands: the equator, the middle latitude and the polar region.

In terms of latitudinal distribution, particles are undoubtedly different.

Looking at all the Tables of the outputs, there is a clear latitudinal variation in both the stratospheric and tropospheric particles.

The equatorial zone is a region of consistently high clouds and thick haze. In this case our model is not able to reproduce the measured signal over the entire instrument

range, anyway we found that the size of the particles is bigger than at other latitudes. Both stratospheric and tropospheric particles are located higher in altitude and looking at the $5\ \mu\text{m}$ images, this region seems not to be populated with clouds but an uniform sheet seems to cover the region, possibly because of strong zonal wind shear. Since the scattering density is proportional to the aerosol number density and the backscattering coefficient either of these or both, must be larger in the tropics than at middle latitudes (assuming a similar chemical composition).

The aerosol number density depends strongly on the number density of available condensation nuclei. The latter number density could be relatively large at tropical latitudes because of a relatively large influx of dust-like particles from, for example, micrometeorites or precipitation of ring particles [49].

At middle latitudes before near -60° the first principal variation occurs.

Here, our model predicts smaller particles with the base of the clouds located at lower pressures with respect to the equatorial region. The opacity become lower for both the stratospheric and tropospheric clouds.

At this latitudes, atmospheric areas with a complete different deep clouds structures show the same spectral behavior in the solar part of the instrument range between near $1\ \mu\text{m}$ and $3.2\ \mu\text{m}$. The different deep clouds structures are well visible in the thermal range between $4.4\ \mu\text{m}$ and $5.2\ \mu\text{m}$ and in the images at $5.1\ \mu\text{m}$ as well.

The base clouds pressures after this boundary at about -60° increase with latitude moving to the South Pole, with the pressures in general being bigger than those before the boundary for both the stratospheric and tropospheric clouds.

After that boundary, the size of the particles becomes smaller and the optical thickness decreases in the analyzed region.

Besides pressure variations in the upper cloud layers, we also find for that particular regions before the boundary, the highest opacity for the deeper clouds than the other observations.

At polar latitudes, for the analyzed image the pressure of the stratospheric haze appears to increase, the model shows an equal set of parameters for all the simulated spectra of every ROIs. It seems again that an uniform cap made of a thin stratospheric haze covers the southern polar regions.

The tropospheric clouds extend probably lower than the same clouds at other latitudes and the same values for the size of particles at mid-latitudes after the boundary at -60° are found.

The results of this work seem to support the idea that our model is able to reproduce the signal of the instrument and give indications about some physical constraints of the vertical aerosols and clouds profile inside the range of the parameters fixed *a priori*.

As said before, the retrieved vertical structure of the atmosphere and its latitudinal variation must to be considered only as the best set of parameters that fit the actual data.

We can say nothing about the actual size, particles shape, and/or pressure levels of the upper stratospheric haze or the tropospheric and deeper clouds. Moreover, just to test the model we consider only one observation for every planetary bands, and the outputs can't be really considered as a general behavior.

As future work, we obviously plan to make the model complex, introducing other

cloud layers, as the water cloud at very deep levels where is expected to be as pointed out by other studies [57].

In order to simulate in a better way the region near $3\ \mu m$, where we are not able to fit the actual spectra because the masking by a foreign contaminant of the ammonia fresh ice, the introduction of different mixtures of ammonia ice is planned as well.

Even if our model is based on simplifying assumptions however, our results are in agreement with the results obtained by other studies, and this agreement is remarkable considering the very different techniques used in the different works and the most complexity of the other models.

Despite the title of this thesis the model has been applied to the Saturn's atmosphere only.

The reason lies in the low spatial resolution of the VIMS images during and after Cassini's closest approach to Jupiter on December 30, 2000.

The images are not spatially resolved enough in order to test our model.

In the Jupiter case in fact, the model was not able to give reasonable values for different clouds profiles because too low spatial resolution of the VIMS images.

This is probably due to low model sensitivity and the strong assumptions we made.

The radiance of every pixel in fact, was a signal averaged between very different parts of the atmosphere and the application of ROIs to discrete and uniform areas discriminating different aerosols and clouds vertical distributions would not have been an easy task.

However, this model can be applied to data from other future mission as well, where the quality of the images would be comparable to the ones with VIMS at Saturn.

In view of the Italian participation to the NASA New Frontiers mission JUNO to Jupiter (whose launch is planned for 2011) in fact, Italy extends its contribution by the addition of JIRAM (Jovian InfraRed Auroral Mapper) to the scientific payload.

The proposed JIRAM experiment is designed to obtain high spatial resolution images of the Jupiter atmosphere and to retrieve its spectral properties between $2.0\ \mu m$ and $5.0\ \mu m$ range.

Thanks to an innovative optical design concept, JIRAM will share a single telescope for the infrared camera and spectrometer: this configuration allows us to obtain at the same time the image of the polar regions of the planet and the spectral radiance over the central zone of the image.

Instrument design, modes and observation strategy will be optimized for operations aboard a spinning satellite in polar orbit around Jupiter.

The JIRAM data will provide new testing for our model, making our code more realistic and flexible for different atmospheres.

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